TQ Analyst Release Notes

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About This Document

This document contains a revision history of TQ Analyst, including new features that may not be included in the User's Guide, resolved issues, and known issues.

Trademarks

TQ Analyst 9.14

- **Build number:** 9.14.0.97
- **Release date:** January 2024
- **Supported operating systems**
  - Windows 10 64-bit
  - Windows 11 64-bit

New Features

Added Composite Component MAXINDEX to Simplify Any PLS-DA Method

A PLS-DA method may be set up in the PLS method type. However, to show the best class requires many composite components before you can see the answer. The new composite component MAXINDEX allows this to be done in one composite component.

Resolved Issues

None

Known Issues

None

TQ Analyst 9.13 Hotfix 1

- **Build number:** 9.13.1.2
- **Release date:** January 2023
- **Supported operating systems**
  - Windows 10 64-bit

New Features

None

Resolved Issues

SNV calculations are incorrect at the endpoints when spectrum is smoothed first

If you smooth or take the derivative before applying SNV, then if you choose the entire spectrum, the SNV correction will be incorrect.

Raman… library limits don’t match expected value (from spectrum registration)
When saving the spectra in csv format, the x-axis is not the same when saving from an OMNIC window where all SPA files are opened or when saving it individually from a separate window. The difference of min-max observed does not correspond to the range the in TQ method.

Known Issues
None

TQ Analyst 9.13

- **Build number:** 9.13.0.292
- **Release date:** April 2022
- **Supported operating systems**
  - Windows 10 64-bit

New Features
Inform users that an external executable is being run
TQ Analyst now warns each user the first time a request to run an external program is made (or example, when a program is run from a toolbar button). If the user allows the external program to run, the warning will not be displayed to that user again unless the program is changed. This warning was added to ensure users are aware a program that could potentially harm their computer is being run with their credentials.

Add composite components for RMS noise calculation and single beam intensity calculation
Composite components for reporting RMS noise from an absorbance spectrum, reporting RMS noise from a transmittance spectrum and reporting the single beam intensity at a location have been added to the Composite tab.

When displaying a report show a blank field when the answer is -1
For Measurement Only methods if the answer for a measurement is -1, then report it as an empty field.

Add commands to clear all regions from a method and to add a region to a method
Add DDE commands `ClearAllRegions` and `AddRegion` to support creating information for the Region tab. This is a step toward being able to fully build a TQ Analyst method from a DDE script.

For the "DeleteSpectrum" and "Select" commands allow them to work on any window TQ Analyst type
This is needed to allow these commands to work from the Region Select window in TQ Analyst.

Allow the "New", "SetMethodType" and "AddComponentToMethod" to run from OMNIC as well as TQ Analyst

These commands already existed for TQ Analyst. Now allow them in OMNIC as well. This is a step toward being able to fully build a TQ Analyst method from a DDE script.

Add command to extract support spectra from a spectrum

Add DDE command `ExtractSupportSpectra` to extract the Ratio spectrum and the Subtract spectrum from the current spectrum, if they are present. Display them into the current spectral window.

Add temperature, pressure and pathlength to the currently selected spectrum

Add DDE command `SetTPPIntoSpectrum` to add the specified temperature, pressure and pathlength into the selected spectrum. This command is available from both TQ Analyst and OMNIC.

Allow concentrations to be read to the Standards table based on the file name of the standard

Add DDE command `GetConcsForStandards`. This will read a text file where based on the file name of the standard it will populate some or all of the concentrations into the Standards table in TQ Analyst.

Allow Similarity Match methods to be added to Combined Mathods

Allow Similarity Match methods to be added to a Combined Methods TQ Analyst method.

Resolved Issues

Calculate peak location needs to give a better value when the height is less than the threshold

When the peak height is less than the defined threshold, the peak location is reported as NaN. For use in ValPro scripts, it is better to return a -1 in this case. This change is made.

TQ Analyst will not open if TQ Analyst Data Security is not installed

The workaround in older versions is to delete "OMNIC_cr.dll" in "C:\Program files (x86)\TQ Analyst". With TQ Analyst 9.13 this workaround is no longer necessary.

Uncertainty values may be shown in a report with Simple Beer’s Law and SMLR methods

Since there is no uncertainty computed for these method types, the uncertainty should never be shown for these methods.

Cannot measure a peak height outside of the original spectral range when using the Sample Single Beam option

In Measurement Only methods it is possible to perform a measurement not only on the current spectrum, but also on the sample and background interferograms for the spectrum and on the sample and background single beams for the spectrum. When the sample (or background) single beam is selected, the resulting spectrum will have the same spectral limits as the original spectrum. We have tests that require measurements outside of that range. In TQ Analyst 9.13, the calculated sample (or background) single beam will be returned for the entire spectral range.

The number of measurements and the number of uncertainties do not always conform when using QuantPad methods

If the QuantPad method uses the composite component option from TQ Analyst, then the measurements and uncertainties will not conform and this will cause an error.

The multiple summary report shows too many decimal digits for the uncertainty

For PLSplus/IQ methods, the uncertainty value in the multiple summary report displayed with many digits. The fix is to show five decimal digits for PLSplus/IQ uncertainty values. The concentration values are reported to four decimal digits.

Program crash found entering component names into a method from a text string

Fixed an issue where the entered component name in the `GetComponentName` DDE command was longer than 63 characters. This wasn't protected in the command.

Did not set component names when adding the first standard to a TQ Analyst method from JCAMP-DX

Allowed the component names to be read from the JCAMP-DX header when a first standard is added to a method.

Possible error fixed in the case where a correction spectrum is applied

This issue is important in the correction to handle when the sample and background are collected from different beampaths. The detection of a single beam is done incorrectly and

Long file titles and file names cannot be displayed on the Standard table in the Standards tab of TQ Analyst

The file titles and file names allowed 60 characters in the Standards table. This is increased by 250 characters in response to some customer issues.

The TQ method does not uncalibrate when the Intercept column of the Measurements tab is changed

This can lead to situations where the settings from the Measurements tab do not reflect the calibration data. Now a change to the Intercept column will cause the method to be uncalibrated.

Potential error in calibration results when missing values is set

The situation where there is a problem is for Known pathlength, Predict pathlength and Internal reference pathlength. In these cases any standards with the missing data value set will not be used properly during calibration.

Known Issues

SNV calculations are incorrect at the endpoints when spectrum is smoothed first

Smoothing adds zeroes at the beginning and ending of a spectrum. These zeroes are then included in the SNV calculation. Add a routine to ignore leading and trailing zeroes when calculating the mean and standard deviation for SNV.

TQ Analyst 9.12 Hotfix 1

- **Build number:** 9.12.1.116
- **Release date:** January 2021
- **Supported operating systems**
  - Windows 7 32-bit
  - Windows 7 64-bit
  - Windows 8.1 64-bit
  - Windows 10 64-bit

Resolved Issues

With Thermo Security installed, TQ Analyst launches for a user that does not have permission

Fixed a problem in how TQ Analyst is launched under Thermo Security conditions. Now honors the access rights specified in Security Administration. Will not launch unless the access rights are allowed.

Known Issues

None

TQ Analyst 9.12

- **Build number:** 9.12.0.108
- **Release date:** October 2020
- **Supported operating systems**
  - Windows 7 32-bit
  - Windows 7 64-bit
  - Windows 8.1 64-bit
  - Windows 10 64-bit

New Features

Add three new options for Multipoint Baseline Correction for QuantPad (or MultiStdCLS) methods

Add Piecewise linear, Spline correction and Autobaseline Correct as Multipoint Baseline options for QuantPad (or MultiStdCLS) methods. Change Quadratic Remove to use either one region at a time or pooled regions.

Add U_INIT and UU_INIT composite components

Write the specified value into the appropriate user and method user position. But only do this if the current value at the position is a NaN. This makes it a way to set an initial value into the user value.

Split the user values into an unsecured group and a secured group of values

To support secured values used in ValPro methods, provide a set of secured user values. These are values that cannot be accessed unless a key is entered. Split the user values into two sets. One set is unsecured (like the current values) and the other set is secured.

Hide composite components when the component / measurement answers are in error

Since composite results may be poorly calculated if the components or measurements produce a bad result, do not show the composite components.

Resolved Issues

Increase the maximum number of classes that can be reported

Increase the maximum number of classes that can be reported from 50 to 80. This supports a customer request.

Baseline items not set correctly in Edit Regions

There was an issue found in the Edit Regions button in the Regions tab. When you clicked on a peak, it would try to update baseline items that weren’t intended to be changed. Changes to the peak location and the baseline have now been separated.

When the answer value is very close to a threshold or acceptance limit, the pass/fail test doesn’t give the result you expect

Improve how answers are rounded when comparing an answer to threshold or acceptance limits.

Calibration results for Ignore standards do not update when the component is changed

Fix the problem where the results for standards that are set to Ignore do not update when you change components in the calibration table.

Multiple Summary does not honor the pathlength that is set for a Known Pathlength type

Not doing this caused an issue when opening a Measurement Only method in Paradigm. The fix was compatible with how the calibration step should run in TQ Analyst / OMNIC.

The three argument version of the PKHGT composite doesn’t give the correct result

Correct the result for the three argument PKHGT composite where the second baseline location is handled correctly. Also correct a problem with the four argument PKHGT composite, also with the second baseline. Make the default baseline "average in range" for PKAREA, PKHGT and PKLOC.

Known Issues

None

TQ Analyst 9.11

- **Build number:** 9.11.0.728
- **Release date:** October 2019
- **Supported operating systems**
  - Windows 7 32-bit
  - Windows 7 64-bit
  - Windows 8.1 64-bit
  - Windows 10 64-bit

New Features

Allow "Attach results to the spectrum" for a Similarity Match method

Allow the option of attaching the prediction answers from a similarity match method to the spectrum that was measured.

Add the "Open Spectra from TSV" menu item to the File menu

Add the ability to open a tsv multispectral file from Nanodrop from the TQ Analyst menu. This allows the TQ Analyst application to more easily support UV/visible spectra.

Open Nanodrop TSV files into the Standards tab

The .tsv extension has been added to the allowed spectra types that can be opened into the Standards tab. This allows the TQ Analyst application to open UV/visible spectra as standards and makes it easier to support building methods from UV/visible spectra.

Provide User Variables that are associated with the TQ Analyst method

User variables (call U values) are available in TQ Analyst, however they are attached to the computer / instrument. The new UU values are attached to the TQ method, so that each method has its own set of variables available for long term saving of values. There is also a new UU_SET composite that allows these values to be populated. To save the new values with the method, the method must be explicitly saved after the values are set. That is, UU_SET does not trigger a save of the method.

Add a special class (or library) entry that will always be reported

Add a special class (or library entry for Search) that will always be reported for Discriminant Analysis, Distance Match and QC Compare. Add a DDE command that will fill the special class or entry for a particular TQ method. After predicting the result will be printed at the bottom of the output table.

DDE command to write the spectrum header to a text file

Add the DDE command `AddSpectrumHeaderToText` to save the contents of the spectrum header to a text file (SpectrumHeader.txt).

Add an alternate name for components or measurements or composites

Support a second name for each component / measurement / composite. This name will be picked up by RESULT software instead of the normal component name. This allows a common name to be defined while also keeping a specific, descriptive component name.

Add DDE command to get the value of a parameter

Implement a new DDE command called `Get` to allow access to any OMNIC parameter. It writes the result to a test file in %temp%. Even when the Get returns an unknown parameter, print out a line into the text file.

Add new diagnostic composite components

Add composite component "OMCOLLECTERR" to give a numerical error if a problem occurred during OMNIC data collect. A zero implies no error. Add composite component "iMODULETEMP" to the set of instrument diagnostics that are available. The will show the temperature of the instrument module.

Add features to the TQScript or DDEScript DDE command

Enhance the TQScript (DDEScript) command with the following features.

- If an error is found when using the `Set` command, continue with the script.
- Do not stop the script if there is an error when the command is set for `polling`.
- Allow the script to continue even when an error is detected with a command. (Some commands already supported this, but now it can be made general.) Insert a `1` at the end of the file name to turn on this feature.
- The double quote will now delimit a comment line. Also can use `\` to indicate a comment.
- Allow repeated runs of a script. If the last calling argument to the command is a number, then this will be the number of times that the text script will be executed.
- Display a message box if the file that contains the script does not exist.
- Rather than passing the file name to the TQScript command, you can enter a single line DDE command (delimited with `[ ]`).
- The input file name passed to the TQScript command is static; making it easier to re-run the identical command.

Add third party MultiStdCLS as a possible and supported Quant method type

Add the ability to open and process quantitative methods created in the MultiStdCLS application.

Install lines into TQSettings and OMNICSettings to support MultiStdCLS application

Add GasQuantDlls section to TQSettings.ini and OMNICSettings.ini to define how the MultiStdCLS application will be seen.

Save composite and baseline correction information to support MultiStdCLS methods

Support the features used by QuantPad for composite components and baseline correction for MultiStdCLS methods.

Do special error reporting for third party MultiStdCLS methods

Thermo Fisher Scientific can't be responsible for identifying the errors coming from the 3rd party quant engine. So this change means that any error from the 3rd party package will be shown in a message box as they are found. Generally this will not happen, but there will be instant feedback.

Add parameters to report uncertainty results and pass/fail results in TQ Analyst

Add `[Quantify TQErrors]` to save the array of uncertainties for components and composites from a TQ Analyst prediction. Add `[Quantify TQPassFailAns]` to save an array of pass/fail results and high and low control limits. Make sure that the pass/fail limits (control limits) are part of the TQ Analyst method before using.

Improve the SELECT DDE command to allow a "CONTAINS" option

Add the `CONTAINS` option to the `SELECT` command. This allows a spectrum to be selected if the title of the spectrum contains a substring that is entered. That way you don't need to specify the entire title … or you can use a title that has a date/time appended.

Save uncertainty results and pass/fail answers as method parameters

Create `[Quantify TQErrors]` as an array of the uncertainties (standard errors) for the components measured in a prediction. Create `[Quantify TQPassFailAns]` as the results of a pass/fail test and the high and low control limits for the components measured in a prediction. Make sure that the pass/fail limits (or control limits) are available before using TQPassFailAns.

Support Average in Range or Min/Max in Range for "Single point baseline correction" as an option to Multipoint Baseline Correction

These are one point baseline correct options for a single point baseline correction. If more than one region is defined, then option 4 will average the answers for the multiple regions. Option 5 will report the minimum of the multiple regions (if peaks go up for the spectrum) and will report the maximum of the multiple regions (if peaks go down for the spectrum).

Enhancements made to support the "Quantify OMNIC Analysis.exe" program

The enhancements include the following items.

- Allow a second level of wildcarding in the path with the last directory.
- Read spectral group files (*.spg) in addition to single spectrum spa files.
- Perform a live TQ Analyst prediction on a spectrum before displaying the results.
- Include or exclude based on the file name or the spectrum title. Previously this feature was limited to the component names.

Provided program to support moving SPA files to compatible SPC format

Create DDE command `ConformToReference`: This will conform a directory of spa and spc files to match a reference spectrum. Conform means data spacing, first x value and last x value will match the reference spectrum.

Add "Minus log sample single beam" to "Use special format" on the Measurements tab

On the Measurements tab, add two options under *Use special format*. The options are **Minus log sample single beam** and **Minus log background single beam**. These are used to convert a single beam measure into a value that is more absorbance like.

Implement spectral reference adjustment before subtraction

Set up an offset to work with the pathlength when the pathlength is the last component predicted. To be valid, the offset must be entered two times… as the two values just before the last component predicted result. This is a very back door way of implementing a reference adjustment.

Write component names into a JCAMP-DX spectrum

Write the component names from the comments section of an spa file into the CONCENTRATIONS section of a JCAMP-DX spectrum.

Retrieve the pathlength, temperature and pressure values from a JCAMP-DX spectrum and load them into a spa spectrum

Read the pathlength, temperature and pressure values from a JCAMP-DX spectrum and write them into a spa spectrum.

Retrieve the pathlength, temperature and pressure values from a spa spectrum and load them into a JCAMP-DX header

Read the pathlength, temperature and pressure values from a spa spectrum and write the values into the header of a JCAMP-DX spectrum.

Load the pathlength, temperature and pressure values into the header comment of a SPC spectrum

If pathlength, temperature and pressure values are available from a spectrum, then write the values into the header comment of a SPC spectrum.

Support compatible read and write of TQ Analyst methods between TQ Analyst (OMNIC) and Paradigm software

Confirm that a TQ Analyst method may be read from Paradigm software. Also if Paradigm alters a TQ Analyst method, verify that it may still be read from TQ Analyst.

Add ability to automatically read a region that includes the entire spectrum for a Measurement Only method

When the region limits are set to either +99999 or -99999, then the region (in the Region tab) will go all the way to the end of the spectrum. This is especially valuable when reading an interferogram where a method can be set to use the entire interferogram regardless of resolution.

Return a set of data points from a spectrum

Return one of more consecutive spectral data points from a spectrum in DDE command. Up to 100 data points may be extracted into `[RESULT ARRAY]` using the `GetSpectrumPoints` DDE command. The points will be tab separated in RESULT ARRAY.

Add options to define how pathlength is adjusted for Nanodrop

Pathlength adjustment for Nanodrop is done from the user interface. However this is a selection that could and should be made thru a TQ Analyst method. Add this to the TQ user interface. There are no active steps that have to be taken in TQ Analyst based on these settings. This is added to the Advanced button from the Pathlength tab in the section named "Pathlength Adjustment during Data Collect."

Resolved Issues

From a macro, do not fail if you try to close a window that is not present

Do not report an error from the `CloseWindow` DDE command when you don't have a current window to close. It was never the intent to make this into a trap for the macro writer.

Unable to write a spectrum back to disk

If any of the parameter sections in a spectrum fail to write, then the spectrum will not save. Now ignore that section and continue to make sure the header section is written. This will save the spectrum, although some parameters may be missing.

An error occurs when you extend beyond the maximum number of components in the Components tab

Improve the Cleanup routine when maximum components (measurements or composites) are found. Also make sure that cannot create a report allowing more than the maximum number of rows (components).

Error occurs when an interference in a CLS method is all zero

This case is unlikely except when an artificial spectrum is generated (e.g. using HiTran). In this case report an erro if an interference part of a pure spectrum is (essentially) all zero.

Automatically set a Measurement Only method to Calibrated when the method is saved

Not doing this caused an issue when opening a Measurement Only method in Paradigm. The fix was compatible with how the calibration step should run in TQ Analyst / OMNIC.

The spectrum file path is not kept when the Multiple Summay - Select Directory command is used

Fix the problem in the Multiple Summary command where the path was not preserved for the spectra selected by the SELECT DIRECTORY option.

Do not allow duplicate names for among components and / or composites

No duplicate component, measurement and composite names are allowed. If any are found, then insert an underscore at the beginning of the duplicate name. Note that there may be MORE THAN ONE underscore if there are multiple "components" with the same name.

Remove any "." from component or composite name

OMNIC Schema has a problem if there is an embedded period (`.`) in any component, measurement or composite name. Any periods are replaced with an underscore (`_`).

Error occurs when the name of the composite component is empty
An error occurred when the component, measurement or composite is empty (has zero length). In that case the offset into the names was off.

Changed peak height range and now the peak height measurement fails
When you would change the range of the peak height measurement to be outside of the range of the spectrum, then an error would occur. This was caused by an invalid hidden value for the peak height range. The issue is not fixed and peak height behaves as expected.

Edited the standards spectral range and now unable to predict valid spectra
The spectral limits for the library spectral range were a interpreted too literally. A slight change was made to the match probably data point location.

Unable to pack a quant method into an AQT file
There was a problem when using the "Pack Method into AQT File" command, but only when the method selected was the currently opened method. In that case the command crashed.

Unable to run Excel from TQ
For some of the summary reports the report is generated and then Excel is supposed to be launched to display the report. Running Excel required a user response after a warning. The warning is removed by running Excel directly rather than by launching the report file.

Error in file where TQ Analyst result answers are written
When a prediction is done, the answers may be written into a text file. The end-of-file character was not written properly.

Measurement only prediction fails when using the Interpolate spectrum option
There was an error when the spectrum was interpolated before performing a Measurement Only prediction. The method erred because it couldn’t access the library associated with the method. Since no library SHOULD be associated with the method, ignoring this test cleared the problem.

For small value pathlengths need three decimal digits
Could change the unit of measure for the pathlength, but this is an easy change to make.

Loading spectra diagnostic has an issue if any component name is longer than 25 characters
The component name may be 32 characters long, but the loading diagnostic has a problem when the length of any component name is greater than 25 characters. The fix is to allow a 32 character component name.

TQ Analyst launches even if the Policy "Ability to run TQ Analyst" is turned off
Corrected problem with security policy implementation for the "Ability to run TQ Analyst" Access Control. TQ Analyst will now issue a warning and then shut down if the user is not authorized to run TQ Analyst.

Known Issues
None

TQ Analyst 9.8 Hotfix 2

- **Build number:** 9.8.2.228
- **Release date:** August 2019
- **Supported operating systems**
  - Windows 7 32-bit
  - Windows 7 64-bit
  - Windows 8.1 64-bit
  - Windows 10 64-bit

New Features

None

Resolved Issues

Unable to launch TQ Analyst with Data Security installed

Both TQ EZ and TQ Analyst failed to open when Data Security was installed. This does not impact instruments running OMNIC Paradigm.

Known Issues

None

TQ Analyst 9.8 Hotfix 1

- **Build number:** 9.8.1.220
- **Release date:** July 2019
- **Supported operating systems**
  - Windows 7 32-bit
  - Windows 7 64-bit
  - Windows 8.1 64-bit
  - Windows 10 64-bit

New Features

Compatibility with OMNIC Paradigm Security installation

When installed with OMNIC Paradigm, both TQ EZ and TQ Analyst can correctly find the security server as

configured by OMNIC Paradigm.

Removed all dependences on ToolBook when installed with OMNIC Paradigm

When installed with Paradigm only the ToolBook tutorials will no longer be available from the Help Menu. However, when installed with the legacy products, these tutorials will still be accessible.

Resolved Issues

None

None

Known Issues

None

TQ Analyst 9.8

- **Build number:** 9.8.0.208
- **Release date:** July 2017
- **Supported operating systems**
  - Windows 7 32-bit
  - Windows 7 64-bit
  - Windows 8.1 64-bit
  - Windows 10 64-bit

New Features

New policies when running TQ Analyst in a data security environment

When running TQ Analyst in a data security environment, the software now supports these new policies:

- Require signature when saving spectrum
- Require signature when saving methods
- Prevent changing directories when saving files
- Disable delete, rename and right-click in file dialog boxes
- Prevent signature meaning entry when signing files
- Prevent cancellation of signature
- Directory for quant methods
- Directory for spectral data

In addition, the "Prevent overwriting of method files" policy has been changed to "Prevent overwriting of files" to support both spectral and method files.

Also "Automatically log off inactive system" has been changed to "Automatically lock inactive system".

The software now allows/supports a secure directory that allows you to save files from the TQ Analyst software but returns "access denied" if you try to modify or delete the files from Windows Explorer.

Add "Single point baseline correction" as an option to Multipoint Baseline Correction

On the Spectra tab, add an option for "Single point baseline correction". This option will compute a baseline offset for each spectrum analyzed and that offset will be subtracted from the spectrum before quantifying.

QuantPad support: Save composite and baseline correction information

This enhances the feature added in TQ Analyst 9.7 Hotfix 1. As part of improving the use of QuantPad methods, a "Save to File" button is found on the Composite tab… but only if the Analysis Type is set to "Undecided". Pressing this button will produce a file with a "qcp" extension. The file may be used with a QuantPad method to add composite components to a method and to define a baseline correction to be done to the spectrum. The composite component information is read from the contents of the Composite tab and the baseline correction information is read for the Multipoint Baseline Correction section of the Spectra tab.

Resolved Issues

Reading a JCAMP-DX failed if a data value is reported in exponential form

The JCAMP-DX reader failed if any of the y axis data values were saved in exponential form. This caused an exception when the reader interpreted an exponential value to be two values. This caused an overflow in the number of data points found. In addition to allowing exponential form, the reader was fixed such that the data value buffer cannot overflow. This also allowed an improvement to how the end of data (indicated by END) is found.

Error if the special format spectrum ratio routine returns a null

This is a highly unlikely, but possible, case where the output spectrum from the special spectrum ratio routine needs attached interferograms but finds none. (The special spectrum ratio routine is where features like "dark correction" and "baseline thru a different beam path" are implemented.) In this error case, an exception would be thrown at the end of the routine. This situation is now identified and handled.

Known Issues

None

TQ Analyst 9.7 Hotfix 1

- **Build number:** 9.7.1.179
- **Release date:** April 2017

New Features

Perform Temperature/Pressure correction before items from Corrections tab

Temperature and pressure correction have always been done following the post analysis corrections indicated in the Corrections tab. There are cases when it would be better do temperature and pressure correction before the polynomial corrections. This may be done using the new checkbox from the Advanced button of the Pathlength tab.

Simplify how first-time logic might be applied to set up a time zero quantitative value

Add a DDE command `DeleteTextAnswerFile` that can be used to indicate that next time that a measurement is done it should be considered a time zero result. That is done by using the Znnn composite values and removing any earlier values of these results. The next measurement therefore is the first in the list.

Add ability to report spectrum time and date when the spectrum is measured

Add several composite components that support reporting the time and date that a spectrum was collected. "CLCTTIME" and "CLCTDATE" indicate the time and date that the spectrum was collected. The time is reported as HHMMSS and the date as YYMMDD. "CURRTIME" and "CURRDATE" are available to indicate the current time and date. If you add an "X" to any of these composite component names (e.g. "CLCTTIMEX"), then the values are reported in a format more easily plotted. The time is reported as SSSSS where this is the number of seconds since midnight and the date is reported as YYKKK where KKK is the number of days since Jan-1 of the indicated year.

Add composite components for reporting the interferogram amplitude

Add two composite components that will display the sample interferogram amplitude for the interferogram attached to the spectrum being measured. These composites are called IFGMAX and IFGMAXMIN. IFGMAX reports the amplitude of the larger of the positive going or negative going interferogram peak. IFGMAXMIN reports the peak-to-peak size of the interferogram. Also add the equivalent (two) composite components to display the background interferogram amplitudes. These composites are named IFGBKGMAX and IFGBKGMAXMIN.

Allow non-TQ Analyst methods to run Quantify Sequence or Map

Allow non-TQ Analyst methods (e.g. QuantPad methods) to run the Quantify Sequence or Map diagnostic. This is allowed if there are no methods visible on the TQ Analyst display. That is, you must close all methods visible in the TQ Analyst main dialog. At that point you will be able to choose a non-TQ Analyst method when you execute the "Quantify Sequence or Map" diagnostic.

Allow composite components to be added to a QuantPad type method

Allow composite components to be added to any QuantPad type method. The components will be found in a ".qcp" file with the same name as the method. The composite components text file may be written when you open a QuantPad method into directly into TQ Analyst. This will make an attempt to create a TQ version of the QuantPad method. But on the Composites tab, you will have the ability to save any selected composite components from a "File Save" button.

Add composite components to select which of several subtraction result is reported

Add two new composite components DIFFMIN and DIFFMSUB. DIFFMIN will have the syntax DIFFMIN(A,B1,B2,B3…) which will perform the subtractions A-B1, A-B2, A-B3, … and report the difference that has minimum amplitude. The arguments to DIFFMSUB are the same and it will report the subtrahend (B1,

B2 or B3) that gave the minimum amplitude difference. These composites are valuable when the same method would be used to report a difference where several subtrahends might be correct for different instances.

Update a number in a composite component formula item in place within a TQ Analyst method

Two new DDE commands are available.

Command	Syntax	Description
GetCompositeNumber	`[GetCompositeNumber nCompos]`	`nCompos` is a valid (one-based) composite number in the current method. If the formula for this composite component is a simple number, then it is reported into `Result Current`.
UpdateCompositeNumber	`[UpdateCompositeNumber nCompos fNewValue]`	`fNewValue` is the new number that will be loaded into the `nCompos` composite component. This value will only be loaded if the current composite formula is a simple number. This is a way of replacing / updating a number that is a composite formula in place within the current method.

Quantify Sequence or Map will work with a series file created in OMNIC

The Quantify Sequence or Map in the Diagnostics menu had always worked for sequence (series) files created in RESULT. However it was not effective for files with the srs extension created in OMNIC.

Add composite components FILEOMNIC and for FILERESULT

These new composite components read the i-th (one based) value from the file with the same name as the method. If FILEOMNIC(i), then the file is assumed to be found in "C:\My documents\OMNIC". If FILERESULT(i), then the file is assumed to be found in "C:\RESULT Data\Archive".

Add composite components to report statistics for the residual spectrum left by a quantitative analysis

New composite components "RESIDUALRMS", "RESIDUALMAX", "RESIDUALMIN", "RESIDUALMAXLOC" and "RESIDUALMINLOC" have been added to report values from the residual spectrum left by a PLS, CLS or PCR method. A one-based argument value will be added to the composite component for a PLS method since a different residual is produced for each component. Since the rms, max and min values may be small, if you add 1000 to the argument, the reported value will be multiplied by 1000.

Resolved Issues

None

Known Issues

None

TQ Analyst 9.7

- **Build number:** 9.7.0.27
- **Release date:** September 2016

New Features

TQ Analyst version number jumped to TQ Analyst 9.7

The TQ Analyst version number was jumped to 9.7 to agree with the version of OMNIC that is being released at the same time.

Complete the support of TQ Analyst with Windows 10

TQ Analyst 9.5 was Windows 10 compliant except for the Tutorials (for the Tour and for the Example Methods). These require the use of ToolBook 11.5. OMNIC 9.7 and TQ Analyst 9.7 both are configured to run with ToolBook 11.5.

Resolved Issues

Running TQ Analyst with a 2 cm^{-1} spectrum and a 4 cm^{-1} TQ method causes a failure in the analysis

This feature was supported in TQ Analyst 9.5, however the methods that were used did not require that the full spectrum fit or the region fit be computed.

Standard deviation (STD) composite component gives incorrect results

If the results from previous TQ analyses are used in the equation for the standard deviation and the first component from the TQ analysis is part of the standard deviation equation, then the incorrect number of measurements in the standard deviation may be used to compute the result.

Correct the component name labels in the "Quantify OMNIC Analysis" (or "qPro OMNIC Analysis") program

The column component name labels in the spreadsheet for "Quantify OMNIC Analysis" may be incomplete when results from multiple TQ methods are found in the directory being searched. This is now done correctly and the correct and complete list of components (and composites) is listed. Also added the ability to filter -999 answer results and treat them as if no component was computed.

Measurement of TQ method from RESULT software fails

If the TQ Analyst method was a measurement only method with no measurements and any number of composites, then including that method in a RESULT workflow will cause a failure.

Known Issues

None

TQ Analyst 9.5

- **Release date:** August 2016

New Features

TQ Analyst is supported on Windows 8.1 and Window 10

TQ Analyst software is supported on Windows 8.1 and Windows 10.

Do not Normalize the spectrum before predicting

For a Measurement Only method, add a checkbox to the Measurements tab. The text says "Do not Normalize the spectrum before predicting." This allows a user to control whether the input spectrum may be altered before the predicting is done.

Allow all the files associated with a TQ method to be written into one file

Two new commands are added to the File menu. "Pack Method into AQT File" will take all of the files associated with a TQ method and pack them into a single file with an ".aqt" extension. This is useful to move a method from one computer to another. There is also a new command "Unpack Method from AQT File" which will reverse the process and break the AQT file back into its operational files.

Add special, specific Composite component types to support the ND One application

Two new composite component types (SPCL_NAPRO and SPCL_GUAN) have been added. These commands have very special rules that combine many other composite calculations. They are not useful outside of their intended application.

Add special, specific Composite component types for measuring the top of a peak

Add two new composite component types that are very specific and special.

1. Measure the slope at the top of a peak
2. Measure the slope of the baseline under a peak.

Add new Composite component types that mimic measurement only for quantitative methods

Add composite component types that mimic measure only values. The types added include PKAREA (peak area), PKHGT (peak height), PKLOC (peak location), PKMIN (minimum value in a range) and PKMAX (maximum value in a range).

Add new Composite component to indicate if instrument diagnostics pass

Add the composite component measure called INSTRUMENTDIAGS. This will measure instrument diagnostics

(near the time of the data collection) and report if any of the tests fail.

Add new Composite component to test if a value lies in either of two ranges

Add the composite component called IF2RGN. This will return one value if a measurement falls within either of two value ranges. It will return a different value if the measurement is outside of either range. This is useful for determining if a number passes or fails.

Add new Composite component to display the laser frequency of the current spectrum

Add the composite component called LASERSPECTRUM. This returns the laser frequency at which the current spectrum was collected. In the best case this is taken from the attached sample interferogram, but in the absence of the interferogram being attached to the spectrum, it will return the laser frequency of the current spectrum.

Add "Peak width at half maximum" for Simple Beer's Law measurement

"Peak width at half maximum" is added as an allowed Region type for Simple Beer's Law.

Need to be able to display a concentration profile from a .cnc file

Add a DDE command `[ <invoke> CNCToConcSpectra <filename> ]` to take the contents of a cnc file (from Series / Sequence) runs and produce concentration profiles for the components reported.

Add a reporting option to "Report as zero if value is not above the detection limit"

On the Component or Measurement tab, add an option to the items in the Report column. The new option will set the answer to zero if the calculated answer is less than the detection limit. The detection limit for a PLS method is defined as 2.5 times the uncertainty. For a CLS method it is defined as 1.5 times the reported standard error (which is already two times the estimated standard deviation).

Allow slope/intercept and RMSE to appear simultaneously in the calibration dialog

On the Calibration Results display, allow the case where the slope / intercept and the RMSE values are displayed simultaneously on the display.

Distance Match works for a one-class problem if the Constant Deviation option is set

If the Constant Deviation option is set in Distance Match, then allow the method to be successful even if there is only one class.

Add a weakly weighted Concentration Weighted PLS option

Add a weakly (or Poisson) weighted concentration weighted PLS option on the Other tab for a PLS method.

Time of data collect column added to the Multiple Summary report

The time that the spectrum was collected was added as a column in the Multiple Summary report.

Add the ability to define optional text files for answers for Composite calculation

Add the ability to define optional text files for answers (based on a "channel" number) for Composite calculations. This method is available but hidden in normal use.

Add an invalid value for a Composite for use in subsequent calculations

If a composite component is found to be -999.0, then assume that the value is invalid. This will permit logic to be performed on a composite value. This would usually be used when read from a file by the composite component.

Change how the value assigned for zero concentration is defined for Weighted PLS

Zero or near zero concentrations are a problem for weighted PLS. These values were replaced by a set value in previous versions. However the scale of the concentrations needs to be taken into account as we set the default value. Base it on the number of decimal digits requested for this component.

Modifications to the "Quantify OMNIC Analysis" (or "qPro OMNIC Analysis") program

Enhancements to the "Quantify OMNIC Analysis" program include:

1. Make component name comparisons into a "Containing" function and not an "Equal" function
2. Allow sorting with AND or OR functionality in the component names to limit the spectra reported
3. Allow a wild card in the name of the directory searched
4. Add the ability to report only the spectra collected in the last xxx hours

Set up Scaled Pure Spectra for special applications

Support a scaled pure spectrum for a method where all of the standards are pure standards (only contain one component). This was done for a special application.

Save the type of Special Format used with the measurement answers

A Measurement Only method may be set up for not only work on the current spectrum , but also may be made to work on the attached interferograms or the single beams calculated from the attached interferograms. These are among the Special Formats available. When answers are saved to the spectrum, it is critical to know the format that was processed and this information was added to the spectrum in the section for the TQ Analyst method that generated the answers.

Only save answers to the spectrum if the spectrum is an .spa file

Do not try to save answers to a spectrum unless the spectrum is saved to an .spa file.

Add the ability to validate the standards in a Search standards method

Add a "Validate Standards" button to the Standards tab of a Search Standards method. For a calibrated method, this will predict each standard against the method and report the best two matches. The first hit should always be the standard itself and the second hit should have a match value different and inferior to the first hit. This validates a method for use in a regulated environment since the method is self-consistent and no spectrum appears more than once

New Composite components to report values for instrument diagnostics are available

Ten new instrument diagnostic composite components have been added. They are iPLUS5, iPLUS12, iMINUS12, iLASERX, iLASERY, iLASERR, iLASCURR (for laser current), iSRCCURR (for source current), iSRCPWR (for source power) and iBOARDTEMP (for board temperature). These values will only be read from the instrument if the TQ Analyst method is called within five minutes of the time that the spectrum is collected. Otherwise, if the values have not already been read from the instrument, the values will be filled with a default

value. If the acceptance limits are not filled when first used, the limits read from the instrument will be set into the method.

Resolved Issues

Major cleanup of how numbers as strings are handled using international decimal separators

Carefully check DDE and drop-down responses to verify that the correct international decimal separator is found and used. This means that macros (for example) written in English will work in Germany or France where the decimal separator is a ",". However, the reverse is NOT true at this time.

Cross validation does not apply the Correction to its final result

Cross validation stops calculating immediately after the predict step. If a post analysis correction is performed, then that is not reflected in the cross-validation results. Change this so that the SAME CORRECTION is applied as for the calibration step.

Composite User values are not always recognized when a change is made

When switching between TQ Analyst and OMNIC, changes to the User Composite values are not always recognized. Loading the options (where the User values are saved) as a step in opening a new TQ method will solve this.

"Run TQ Analyst Script" fails when the curly quotes are used in the text file

ASCII character 147 is a curly open quote and ASCII character 148 is a curly close. These were not recognized as quote characters in a TQ Analyst script. They are now recognized.

"Run TQ Analyst Script" fails when there is a ";" embedded in a command

The semicolon is the separator between commands in the same line of a DDE statement. The "Run TQ Analyst Script" command did not distinguish between a semicolon between commands and a semicolon embedded in a text string argument.

If a spectrum is squared, the start and end of the spectrum are not handled correctly

If a spectrum is squared or logged as part of a smooth or derivative operation, then the end points of the spectrum are not handled properly. The smooth or derivative was not done at the ends of the spectrum.

No pressure correction if temperature is not changed

Handle the case where only one of the temperature or pressure is changed and the other appears to have a zero value. In that case set the other value to be the same as the reference value.

Double clicking on a TQ Analyst method causes a crash of the computer

When the full path file name of the TQ Analyst method is very long, the double click Open of the method caused a crash. This situation was handled and the method can now be opened.

Incorrect calibration if there are missing values in the concentrations

If the first component in a method contains spectra with missing values, then the calibration is incorrect. This caused the standards to be offset and the wrong concentrations were assigned to the calibration spectra.

Component set to "Log, but not report", but it still reports
The "Log, but not report" was not implemented correctly.

Multiple copies of the TQ Analyst answers are attached to the spectrum
There are multiple commands that will write the answers to the spectrum. Make sure that the answers are only written the first time.

The Mahalanobis distance values being reported as a composite component are not correct
The number of terms used for the M-distance calculation was increased from 24 to a much larger number. The number depends on the number of factors in the data.

The Norris first derivative calculation has a problem when the gap is zero
The Norris first derivative produced for a segment of 5, gap of 0 is identical to the first derivative produced for a segment of 5, gap of 5. There is an error in the smoothing vector that is produced when the gap is 0 (but only for a 1st derivative).

This will **not** affect a method that is already calibrated. However if a change is made on the Spectra tab and the method needs to be recalibrated, then the calibration will change. If you need to have the old calculation, then add these lines to OMNICSettings.ini and TQSettings.ini.

```
[QuantSetup]

LegacyNorris1D=1
```

This reverts to the original calculation.

Unable to read a JCAMP-DX (multi-)file
This was a case where the only one spectrum was present in a JCAMP-DX multi-file format. This special case will now work.

Unable to read an old QuantIR type method
There was a problem when the QuantIR method was read, but the standard library had been saved already.

On rare occasions the spectrum that had its background collected on different beampath could not be corrected
The routine to do this did not handle all of the situations for extracting the single beams from the correcting spectra.

The Region tab does not appear with my method
This occurred if the method had Protected Standards, a feature added in SP4.

Suggested factors exceed the number of calculated factors
Do not allow this situation.

Cannot save answers to the spectrum for a Grams PLSplus/IQ method
There are applications where this is required, so it was fixed.

Change how Raman spectra are normalized
Raman spectra are now normalized ignoring the laser excitation frequency and the fact that the spectrum is reversed. This is done to provide compatibility / consistency for .any laser excitation frequency.

Setting Number of Matches to Report in Search to a large number caused a crash in TQ Analyst
This maximum values of matches to report was never intended to be unbounded. The same is true of the number of classes to report for Distance Match, Discriminant Analysis or QC Compare Search. A change was made to restrict these values to lie in the range from 1 to 50.

The Cancel button on the Digital Signature dialog does not cancel the writing of the signature
The logic for writing the digitally signed spectrum was incorrect and this has been fixed. The spectrum was always signed.

Known Issues
None

TQ Analyst 9.4

- **Release date:** January 2014

New Features

Create concentration (answer) profiles and display spectra and attached reference spectra for a collection of spectra
Read a directory of spectra that have concentration data written in their headers. Display the spectra and create concentration profiles for the components. If the spectrum has a reference spectrum or an auxiliary spectrum attached, then display it too.

Allow the standards in a TQ Analyst method to be protected
Allow the standards in a TQ Analyst method to be protected. This prevents any of those spectra from being deleted or saved. Allow a copyright message to be attached to that method.

Save a subtraction reference with the predicted spectrum
Add the ability to attach a reference spectrum (when a subtraction is performed from the Spectra tab) to the predicted spectrum. This keeps everything needed to produce the result within the predicted spectrum.

Measure the Mahalanobis distance for each spectrum predicted

Add a Mahalanobis distance diagnostic to be computed with each PLS, CLS or PCR prediction. Measure the M-distance from the spectrum to be predicted to the calibration standards.

Resolved Issues

Unable to read csv files generated by the Unscrambler

The problems were in the empty fields - especially at the start of each line - and the length of each line in the csv files generated by the Unscrambler.

When reading a set of csv files only the first spectrum honors the x-axis setting specified

The issue was that the x axis setting was not being remembered if "OK to All" was selected in the Open CSV files.

Answers are not the same if spectrum measured in PLS or as part of a Combined method

Do not alter the data spacing of a prediction spectrum if in a combined method. Let the child do all of this.

Standard spectra in the spectral library go crazy near the endpoints

When a new standard spectrum needs to be extended (it doesn’t span the spectral range of the standard library) it may be necessary to fill with zero, rather than interpolate to the end. Especially important if the start or the end of the spectrum is filled with noise.

Showing the uncertainty in a Multiple Summary report not supported

Show the uncertainties with the predicted values based on the check box in the Report tab.

Lock up when setting the data collection parameters assigned for a TQ Analyst method

This routine could lock up while trying to compute the levels of zero filling if the spectrum didn’t have respts or ssp set.

A TQ Analyst method becomes uncalibrated when a subtraction reference is not found in OMNIC

Make sure that the method does not uncalibrate when this situation is found from OMNIC.

The temperature and pressure values are not correctly updated when a TQ Analyst method is opened in OMNIC with Gas Quant present

Make sure that the temperature and pressure values are updated properly when changed on the special Gas Quant Quant Setup screen.

Known Issues

None

TQ Analyst 9.3

- **Release date:** September 2013

New Features

Region Select on Region tab honors settings from Spectra tab
Spectra shown when you are doing Region Select from the Region tab now honor the settings made on the Spectra tab for derivatives and smoothing. In past versions this was only supported for Measurement Only methods, but now it has been expanded for all method types.

Data Collection parameters are saved with the TQ Analyst method.
The data collection parameters used to collect standards are now saved with the TQ Analyst method. Currently these are only accessible through DDE, but this could be used to set how unknowns should be collected.

Composite Components constants may now be written in exponential form
The exponential form may not be used as an argument to a composite function, but that may be accomplished by creating a separate composite component and then that value may be used as the argument to a composite function.

New composite component type called IFPASS
IFPASS is defined as a new composite component type to select between options based on whether a test has measurement / component is reported as a pass. The format is "IFPASS (A, Cnotest, Cpass, Cfail)" where A is a pass or fail.

New composite component type called IFTRI
IFTRI is defined as a new composite component type to select among options based on if a value falls within a range of numerical values. The format is "IFTRI (A, Blo, Bhi, Cbelow, Cin, Cabove)" where A is the number being checked and Blo and Bhi are the limits being tested.

New composite component type called MEDIAN
MEDIAN is defined as a new composite component type to report the middle value from a list of values in the argument list.

Add squared spectrum options as Data Formats on the Spectra tab
On the Spectra tab in the Data Format drop down, add options "Squared spectrum", "Squared 1st derivative" and "Squared 2nd derivative". These are useful to highlight spectral features on a spectral map.

Add new Special Format options on the Measurements tab
Add items "Spectrum as absorbance" and "Spectrum as transmittance" to force the format of the spectrum being measured. Also add two very special formats to allow the background or sample single beam to be corrected for atmospherics before being measured. This latter feature is only used in a special customer case.

Change menu item to "PLS Beta Coefficients"
Change the menu item from "Regression Vectors" to "PLS Beta Coefficients". Also add the mean calibration spectrum into the first pane of the beta coefficients. This gives a point of reference to the beta coefficients.

Add the ability to do an auto-reference subtract

On the Spectra tab, add the ability to do an auto-reference subtract. Currently the only options for auto-referencing are performing smoothing on the spectrum and then either subtracting or dividing the smoothed result from or into the original, unknown spectrum.

Allow Known pathlength for Measurement Only methods

Allow Known pathlength type for Measurement Only methods. Also for Known pathlength and Measurement Only, add the ability to set a "reference" pathlength. You perform a measurement at a particular pathlength. If instead you had a device with THIS pathlength, this is the answer or answers that you'd expect.

Add ability to define the last component result as a pathlength for future use

Add the ability to write the last result (the last component or, if there are composite components, the last composite component) into the spectrum as the pathlength metric for this spectrum. That would allow that value to be read or used later.

Resolved Issues

Remove Validation from the right click menu for Leverage and Cross Validation

Remove Validation from the right click menu for the Leverage display. Remove Validation from the right click menu for the Cross Validation display.

Concentrations not being read from a JCAMP-DX spectrum

Allow additional options for spacing in the format of the CONCENTRATIONS line from JCAMP-DX.

Answers not being reported correctly using ANSWS2F and ANSWF2S composite components

Fix problems in how ANSWS2F and ANSWF2S are implemented. Make sure that the answer is saved before it's written to a file.

Unable to add standards to a TQ Analyst method without getting an error

There was an obscure problem possible if adding standards if no components or classes had been defined prior to adding the standards.

Incorrect error message converting a PLS method to Measurement Only

If you convert a PLS method into a Measurement Only method, a warning message is reported. This is a false message about standards that aren't needed in measure only.

User password might be exposed

In a very special situation it was possible that the user password might be exposed for a protected method.

Ratio to %transmission setting on the Spectra tab didn't get saved with the method

Selecting "Ratio to %transmission" or "Ratio and convert to absorbance" on the Spectra tab didn't force the transform to be done. Another change had to be done at the same time or else the change wasn't saved.

Changing to Savitzky-Golay smoothing didn't get saved with the method

If the only change that you make in the Spectra tab is to change between None, Savitzky-Golay smoothing and Norris derivatives or their parameters, then this did not turn on the need for spectral correction. This could

result in a method that did not perform as expected.

Incorrect Pass/Fail results are reported
Pass/Fail results are not reported for the correct components. This occurred when some component do not have pass/fail tests and other components do. The count of pass/fail results got mismatched with components.

The results reported in the spectrum information are confusing
Improve how the results of the analysis are printed in the spectrum information. Put header info and TQ method name information into the results. This continues the improvement started in the last service pack release.

Full width at half maximum answers report a problem
Fix a potential problem when measuring the full width at half maximum value. This requires at least three points in the spectral region being measured. It was possible to set up a region to search that had fewer than three points. That is no longer possible.

Incorrect peak heights are measured
If a peak height was being measured and the top of the peak was such that it was perfectly flat across the top, then it was possible that an incorrect height would be returned.

Discriminant Analysis result not reported properly in a Combined Method analysis
Embedding a discriminant analysis result in a multi-method analysis caused a problem caused an incorrect value to be reported.

Component names for a Combined Method analysis are not reported in a series run
OMNIC Series runs that report TQ Analyst methods use the component abbreviation to represent the component name. That feature was not supported for Combined Method analyses.

Known Issues
None

TQ Analyst 9.2

- **Release date:** December 2012

New Features
"Combine Multiple Methods" analysis method added
A new Quantitative Analysis type has been added and it is called "Combine Multiple Methods." This type allows you to combine multiple quantitative, discriminant analysis and measurement methods into one method. This is especially useful when you wish to combine the prediction results using a Composite component. In addition to supporting TQ Analyst Quantitative and Measurement method, this also supports PLSplus/IQ methods.

Remove the bias of an outrageous data point in mean centering and variance scaling

If a particular value in a spectrum is much too large, close to a NaN, then ignore it when calculating the average spectrum used for mean centering and variance scaling. This unexpected case was found in customer test spectra.

Add ability to read spectral groups when adding standards from the Standards tab

In the Add Standard button on the Standards tab, the ability was added to load a spectral group or groups.

Determine and report the files needed for a particular TQ Analyst method from DDE

From DDE the ability to determine the file names of all files that need to be associated with a TQ Analyst method was added. This also works for PLSplus/IQ methods. The files are returned in a tab separated list.

Add ability to add all spectra from a directory as standards

Added a command ("Add Standards from Directory") to the Diagnostics menu. This allows you to add all of the spectra in a particular directory to a method. At least one standard must already be in the standards table for this operation to work. This allows a huge number of standards to be added at one time.

Scale the uncertainty values for Composite components

For certain composite operations, allow the uncertainty value to be scaled according to the composite operation. Of course if the uncertainty value is an F-statistic the rules needed to be different than for a standard error.

Add composite component for laser shift

Add the LASDIFF composite component. This returns the difference between the estimated laser frequency (estimated from measurements in the spectrum and "correct" value) and the laser value shown in the spectrum.

Add composite components to exchange answer sections of spectra

Add the ANSWS2F DDE command to take the answer section from a spectrum and write that information to a file. Add the ANSWF2S DDE command to read the answer section from a file and write it into the current spectrum being predicted.

Add an extra search capability without removing mean from the spectrum

Enhance Search to allow a "Percent variance described (no mean removed)" Search Type option in the Other tab.

Resolved Issues

Changing the number of factors used does not persist

In PLS, it is possible to change the number of factors used from the Edit Factors button of the Other tab. However this number is not remembered when you return to the Other tab. This means that you have to manually change them on the Other tab.

When leaving the Standards tab, a change in the method is detected when no value had been changed

When leaving the Standards tab, the logic was incorrect for detecting a change. Even a value had been accessed by not changed, it was possible to think that a value had changed. This case was handled properly in this release.

Unable to remove the spectrum associated with a PLSplus/IQ method after a prediction

The software didn't release the spectrum associated with the PLSplus/IQ method following prediction (or calibration).

Unable to add standards to a TQ Analyst method without getting an error

There was an obscure problem possible if adding standards if no components or classes had been defined prior to adding the standards.

Standard spectrum cannot be shown in View Standards

A particular standard spectrum cannot be shown from View Standards in the Standards tab. It was found that the upper and lower y-axis limits of the spectrum were both defined, but the difference was undefined (a NaN).

User variables were not being updated from a TQ Analyst prediction

It's possible to set special user variables from TQ Analyst composite components. However, this was not working properly because the file where the values are saved was described improperly.

The Performance Index is not being calculated during a method's calibration

Some situations existed where the performance index didn't get calculated as part of the calibration step.

The Multiple Summary command reports extra components without column labels

The Multiple Summary command reported values for all composite components regardless of whether they were to be displayed or not. Some of the values were incorrect in this case. The labels displayed properly for the components that should have been predicted, but the values reported incorrectly.

What happened to "Calculate F-statistic" in Discriminant Analysis?

The "Calculate F-statistic" selection for a one class discriminant analysis disappeared from the TQ Analyst software and it had been used by a customer in an important analysis. This was returned to the software for this release.

Unable to read a JCAMP/DX spectrum created by a competitor

Thermo was unable to read a JCAMP/DX file with a y-axis unit of "Transmittance/Reflectance". This is not in the original JCAMP/DX specification, but is being used in a competitor's software. This feature was added in this release.

Answer section in a spectrum is difficult to read

The format of the answer (TQ Analyst results) section in the spectrum header was difficult to read from the "i" button on a spectral display. The format was simplified for this release.

Known Issues

None

TQ Analyst 9.1

- **Release date:** July 2012

New Features

Do not report pass/fail status for some of the components in a method

If you have a method where you want some of the components or composites to show pass or fail, you are now able to set other components to not report pass or fail. To do this set the high and low control limit to the identically same value. Frequently, but not necessarily this value might be zero.

Multiple Summary working on a series file

From the Multiple Summary command, you can open one or more spa or spg files. This new feature allows you to also open series files to be predicted. Unfortunately, this cannot be done from TQ Analyst, but it can be done from OMNIC. To use this ability, add a command to the Analyze menu of OMNIC. The DDE command should be `[invoke SummaryMultiple]`. When you access this command, you can access series files created from OMNIC.

Add ability to add items to the TQ Analyst menus

The "Edit Menu" command is added to the Edit menu. This allows DDE commands or executables to be added to the default TQ Analyst menu system. The "Open Configuration" command is also added to allow the modified configurations to be saved.

Resolved Issues

Columns don’t line up when Multiple Summary report is opened in Excel

If the quantitative method has composite components and the report is set up to include uncertainty values for each component, then no uncertainty value was displayed for the composite components.

Some of my changes to a method are forgotten when I move to another tab

There are several places where changes to a table must be "registered" before they are accepted. When you change tabs and no changes have been registered, then the information in the dialog associated with the tab is not updated.

On occasion I’m unable to add a standard to the standard table

On occasion I’m unable to add a standard to the standard table. This only happens when I try to add the standard one-at-a-time. It does not happen when I select a group of standards and add at one time. It turns out that the failure occurs when the latest file name is longer than the previous file name. In that case the new standard cannot be added in that session. There is a buffer that is not terminated properly.

Known Issues

None

TQ Analyst 9.0

- **Release date:** June 2012

New Features

Add the ability to report the skew of a peak

Add a region type that is "Peak skewness (asymmetry)". This is the difference between the half width on the high frequency side of the peak minus the half width on the low frequency side of the peak.

Add the ability to enter a known or target value for a measurement in Measurement Only

Add a checkbox on the Measurements tab for Measurement Only methods. In the Measurement Limits section, "Use target or known value" is available. When checked you are able to enter a target value for the value being measured. This may be accessed or reported as TRUEVAL(.) in the Composite.

Add ability to compute a laser frequency correction as a Measurement Only composite

Composite components LASER and LASCORR are provided to produce a corrected laser frequency. The arguments are the measurements that are being used for the laser correction. (More than one may be used.) The measured value from the spectrum and the "target or known" value (see previous item) are used to determine the correction. LASER gives the new laser value relative to the laser frequency of the spectrum. LASCORR is the correction factor (as an inverse) for the laser correction.

Display the PLS Regression Values

The factors from PLS may be combined into one PLS regression vector. This ability is added in the Diagnostics menu. The factors are shown in the form of a spectrum where the intensity at a wavenumber value indicates the weight given to that wavenumber.

File name attached to spectrum from View Standards

The file name of the standard spectrum is added to the spectrum header information for each spectrum displayed by the View Standards button. When used with the "Save As - Add File Name to Title…" command, this allows the original file name to be saved with a standard spectrum.

Ratio the input spectrum to a known (constant) spectrum before performing the spectrum measurement

Two new options are available from the Spectral Subtract section on the Spectra tab. The reference spectrum may now be ratioed to the input spectrum to give a %T spectrum or ratioed and then converted to absorbance. Useful when used with a single beam correction spectrum and a single beam measured spectrum.

Modify the Method Description section on the Description tab

The Method Description section of the Description tab is changed to display as individual lines. You navigate by selecting each line. This makes the section more useful since the user controls the spacing of each line.

Allow User variables to be entered for use with Composite components

A new feature is available from the Options command in the Edit menu. A new tab called User Values is present. This allows you to specify variables U1 thru U25 which are system (computer) specific and may be configured on a user's computer. These values may be included in a formula or as an argument in a Composite component calculation. This required that the options.top file be moved to C:\My documents\OMNIC.

Numerical values may be used as arguments for Composite components

Number constants may be used as an argument in many of the Composite component functions. For example SUM(A,12.0) will compute the sum of the first component value and 12.

Uncertainty values attached to Composite component values

There are some situations where the uncertainty value may be directly copied from the Component to a Composite result. For example if you use a composite to select the component value which has the smallest uncertainty, then the uncertainty of the composite will be the uncertainty of the component that is reported. When available, the uncertainty is attached to the composite result. Otherwise a zero is returned. No error propogation is done since the form of the uncertainty is not known by the composite component.

Attaching component and measurement values to the spectrum

For quantitative and measurement methods, there is a new option in the Results section of the Report tab. The option is "Attach results to the spectrum." This attaches the answers to the spectrum in a new file section that may be accessed. Warning and alarm limits may also be saved if checked on the Components / Measurements tab.

Add a Log only reporting option for components and measurements

There are situations when you want to save a value into the "tqinput" text file, but don't want to report the value. There was no way to do this and it's necessary to produce simple versions of composite components like, for example, SLOPE or AVERAGE. This provides a new Reporting option that may be set on the Components or Measurements tab.

Report the F-ratio as the uncertainty for a PLS or PCR method

There is a selection of the Other tab where you may specify that you wish to report the F-ratio as the computed Uncertainty for a PLS or PCR method. When this selection is made, all references to PLS or PCR Uncertainty will report the F-ratio instead.

Unscaled correlation may be used to measure search similarity in QC Compare

The Other tab now allows you to set "Unscaled correlation" as the Search Type. This gives a measure where a difference in baseline will not be removed and therefore will contribute to the similarity measurement.

Uncertainty added to the Multiple Summary report

If you want the uncertainty for each measurement added to the Multiple Summary report, then you need to add a line to the tqsettings.ini file. If you add a line "Uncertainty=1", then subsequent times that you run the Multiple Summary report, you will display the uncertainty value also.

Add ability to secure a TQ Analyst method

The ability to restrict use of a TQ Analyst method based on instrument serial number was added. In this scenario only spectra collected on an allowed list of instruments may be measured with a particular TQ Analyst model. This is model dependent. The model may also be set up to expire after a defined time period. Using the method security feature requires an independent software routine to set up the TQ Analyst method.

Use PLSplus/IQ methods in both TQ Analyst and OMNIC

PLSplus/IQ methods may only be used in TQ Analyst with the "Combine Multiple Methods" analysis type which is not yet visible. It is also easier to use PLSplus/IQ methods in OMNIC. You may select a .cal file from the "Quant Setup" command in the Analysis menu and then use the Quantify command to predict results from a spectrum. This has always been available. However if you now have a spectrum taken from the calibration set of the PLSplus/IQ method and save it as an spc file with the same root name as the method, then you can predict any spectrum (with compatible spectrum range) from OMNIC.

Resolved Issues

Errors when there are more composite components than measured components

Fixed an error when saving and displaying results when there are more composite components than there are measured components.

Error when adding a component

A situation came up where an error was issued when a component was added to a method. This turned out to be a method that had started as a Measurement Only method and was converted to a Quantitative method.

Known Issues

None

TQ Analyst 8.6

- **Release date:** February 2012

New Features

F-ratio output support for components in PLS methods

Add the ability to create an F-ratio value by component in PLS methods and see them as composite components.

Provide pseudo-measurement of pathlength as height or area

Save the height or area as a measure of pathlength for reporting as a composite component. This was previously only possible when a slope / intercept were specified.

Better error messages during calibration of CLS methods

During calibration of CLS methods, show more detailed calibration errors. This is especially helpful with large gas analysis methods.

Increase range allowed in some measurements in TQ Analyst

On region types that allow a percentage of maximum height, open the range to 0.1% to 99.9%. This allowed new test diagnostics to be performed.

Resolved Issues

Export to text file does not save the method.

Export to text file is unable to write to the Program files directory. File permissions are not likely to support this. Write to My documents\OMNIC instead.

Usage values are not retained after changes.

Current, not yet updated changes to usages, classes or categories are lost when a block of items are changed in a table. Save the not updated changes before performing the block set.

Merging standards causes a failure in calibration.

There was an occasional problem during calibration when merged standards were used to group together standards. This might appear as invalid merged standards.

There are still situations where the pressure and temperature are not set properly.

If you do NOT prompt on quantify, there will be an effect from the last standard from calibration. This will cause an error. Also handle a case where the current value might be set to zero. In that case (from RESULT software), use the reference value.

Data spacing not expected for wavelength or Raman spectra when read from JCAMP-DX.

Reading in a JCAMP-DX wavelength or Raman spectrum produced a spectrum with one too many levels of zero filling. This caused mismatches in the data spacing when trying to add a spectrum to a TQ method.

Error reading TQ_PCData3D.txt when running Principal Component Scores 3D Display.

If a particular class in a discriminant analysis method has only two factors, then there aren’t enough factors for a 3-D display. This is now padded to give an extra all zero factor so that the 3-D display will work.

Category information not displayed for classification methods.

No category information was being shown when hovering over diagnostic graphs for classification methods.

Calibration failure when using target standards in an adaptive method.

If the concentrations are not listed in ascending order in the target concentration table, then the method doesn’t function properly. Was unable to sort the concentrations for each target component because of an error.

Slope and intercept cannot be set for a Wafer Analysis method.

Unable to clear the slope/intercept values for a Wafer Analysis method. Information necessary the make the

change had not been defined yet.

Known Issues

None

TQ Analyst 8.5

- **Release date:** September 2011

New Features

TQ Analyst works with Windows 7 64-bit

Confirm that TQ Analyst functions on a Windows 7 64-bit computer. This primarily affected the tutorials which did not function on a 64-bit system using TQ Analyst 8.4.

Resolved Issues

Pressure and temperature not updated properly when quantifying an unknown spectrum.

The settings used in the Pressure/Temp correction tab do not refresh properly when the checkbox "Correct for temperature/pressure" is selected. The values may be taken from the last calibration instead.

Change the calculation for "Calculate Spectral Residual" for a one class Discriminant Analysis.

On the Other tab for a Discriminant Analysis method, the calculation for "Calculate Spectral Residual" is changed. The denominator is now related to the number of data points. This is more in agreement how other packages compute the out of plane distance between an unknown spectrum and the discriminant model, however it is no longer scale independent.

Known Issues

None

TQ Analyst 8.4

- **Release date:** April 2011

New Features

Add new diagnostic command "Principal Component Scores 3D Display…"

The Principal Component Scores 3D Display command displays a rotatable picture up three principal component factor scores or component concentrations. Also supports the ability to set any outlier to Ignore.

X,Y plots are written to the Clipboard.

The X,Y plots (for example the plots on the Calibration window) may be written to the clipboard and copied to other applications. This is done by right clicking on the plot and selecting the menu command to write to the clipboard. The plots can then be pasted into Word, Excel, PowerPoint… X,Y plots include Calibration, Cross-validation, Residual (on calibration window), Principal Component Scores and Leverage

Clicking on a point in an X,Y plot shows information about a standard.

X,Y plots (Calibration, Cross-validation, Residual, Principal Component Scores and Leverage) support a feature where you can click on a point in the plot and see information about the standard represented by that point.

The Usage of a standard may be changed directly by right clicking on the standard in an X,Y plot.

The usage (Calibration, Validation, Ignore) may be changed directly by right clicking on the standard in an X,Y plot displayed from the Diagnostics menu or from Calibration. This is supported from Calibration, Cross-validation and Principal Component Scores and Leverage.

X,Y plots support zooming.

From the Calibration, Cross-validation, Principal Component Scores and Leverage X,Y displays you can box and zoom to highlight a particular area of the display.

Add the ability to define a category for each standard in a quantitative method.

From the Components tab it's now possible to set the ability to "Categorize Standards." This will generate a Classes tab from which categories for the Standards may be defined. The category for each standard is set on the Standards tab. This information is currently used by the 3D Display command.

Add "Calculate Spectral Residual" as an option for the measurement that is computed for a one class Discriminant Analysis.

On the Other tab for a Discriminant Analysis method, add the option to "Calculate Spectral Residual". This is a measure of out of plane distance between an unknown spectrum and the discriminant model.

New Save Spectrum As option to save the spectrum filename into the title.

Allow a spectral group to be saved with the filename of the original file prepended to the spectrum title. This is available from a popup menu attached to the "Save Spectrum As" menu command.

Allow multiple instances of Excel to be open with the Multiple Summary menu command.

Multiple copies of Excel may be open with any of the multiple report menu commands.

Automatically convert standard and unknown spectra to wavenumber.

An option is provided on the Standards tab to automatically convert any spectrum from wavelength to wavenumber as the spectrum is read.

Allow Multiple Summary to run with many more spectra than now.

Multiple Summary may be run on all spectra in a selected directory. This is available as a popup on the menu command "Multiple Summary."

All multiple spectrum Open dialogs are set to Details mode.

All Open dialogs that support multi-spectrum open are now set to Details mode.

Allow the Open Standard dialog to sort the spectra by name or creation date.

From the Edit menu, select the Options menu command. A dropdown will be available to determine how standard spectra and summary spectra will be sorted in the open dialog.

Allow standards to be set to Ignore from the Calibration window.

This is done by including the Ignore standards in the Calibration table. These spectra are listed at the end of the table. The Ignore spectra may also be changed to Calibration or Validation.

Allow the contents of the Calibration window to be saved as text.

A "Save to Text" button is added to the Calibration windows. This will write a text file with the same name as the method that contains the key information from the calibration table.

Make a PLS method more robust to environmental changes.

For PLS methods add a new standard type called "Variational". This type may or may not have concentrations associated with it. More than one instance of Variational spectrum may be defined for a method. Each instance represents a standard run at different conditions. The variation in each instance of variational spectrum is added when determining the model. The variation will make the method more robust to similar changes when the method is deployed. Variational spectra are added as any other type of standard and they are identified in the Standards tab.

Display a correlation coefficient for the Validation Standards.

When validation standards are available, compute and report the correlation coefficient on the plot in the Calibration window.

Add the ability to select the components, measurement or composites that are written to the optional internal text file.

If on the Report tab you choose to write results to a text file, then you can select which results will be written. This can be specified from a new column on the Components, Measurements and Composite table. This column will only be visible when you intend to write the text file.

Add standard concentrations or class name from a file.

Add "Standards Values from File" to the diagnostic menu. This will read a tab separated value file that contains either the file name or the file title followed by the concentrations for the standards. If the method is a classification method, then the second value is the name of the class for the standard. The file names do NOT have to be in the same order as the standards in the Standards table.

Open spectrum files saved as text with one spectrum per line.

The menu command "Open Text Wavelength Spectra" is added to allow a one spectrum per line text format to be read. The first line of the text file contains the wavelength values for all subsequent spectra. Then each following line contains the intensity values for a spectrum measured at each of those wavelengths. These intensities are usually in a "Log 1/R" format. This is a way of entering unevenly spaced data.

Show more digits in Factor Loading table.

Show more significant figures in the values in the table. The values are scaled and the scale is shown in the table column label.

Resolved Issues

Edit terms on the Correction display and then they change.

It is possible to edit the correction coefficients in the Correction display. However these values change when the fit type was re-done. However in fact, none of the columns in the coefficient table should ever be editable… **unless** it's a "Hand Entry" selection. This got confusing because in the past the entries for any of the fitted values could be edited and then they'd change when the fit was redone.

Unable to open a method saved in TQ Analyst.

When you saved a TQ Analyst method to a directory that had a "." in the path name, then you could not open it again in TQ Analyst.

The Standards table doesn't update when you change the Usage of a standard.

If you change the usage of a standard in the Calibration window AND have the Standards tab open, then the Standards table does not update.

The Standards table doesn't update when you change the Usage of a standard. Part 2

If you set an Outlier to Ignore AND have the Standards tab open, then the Standards table does not update.

"Multiple Summary" and "Multiple Quantify" do not work properly if only one spectrum is selected.

The commands only work when more than one spectrum is selected. This is reasonable, but shouldn't be necessary.

Class names are wrong on the Standards tab after the class names are alphabetized.

When you alphabetize the classes, the class values are not transferred to the Standards tab properly.

You may get a crash when you switch from PLS to Discriminant Analysis.

The switch from PLS to Discriminant Analysis caused a crash if the concentration array in PLS had not been set up. This has been resolved.

Some diagnostics give incorrect results when mean centering is selected.

Principal component scores and Spectrum Outlier do not give the expected results when mean centering is used. The cause was that the same spectra were not being used in mean centering (or variance scaling) as were being used in the diagnostic.

The uncertainty value is not being printed for a PLS method.

Fixed a situation where the uncertainty value wouldn't be calculated or printed for a PLS method.

On the PLS calibration window, the number of factors is being reported incorrectly.
The number of factors is reported incorrectly on the PLS Calibration window. All components show the number for the first component.

On the Discriminant Analysis calibration window, the number of factors is being reported incorrectly.
The number of factors is reported incorrectly on the Discriminant Analysis Calibration window. Only the first class is reported correctly for a multi-class problem.

For a one class Discriminant Analysis method, the number of factors is not shown on the calibration window.
The number of factors is not shown on the calibration window for a one class Discriminant Analysis method.

The correct standard is not selected on the plot when I select a standard in the table.
For a discriminant analysis calibration, when you select a standard on the table, the correct standard is not selected on the plot.

The correct number of factors not used for Discriminant Analysis.
The number of factors used for the first class was used for all classes. Change to let each class be determined independently.

Path information not used for Pure Component or Statistical Spectra diagnostics.
For Peak Ratio and Internal Reference pathlength methods, the path information should be used when determining pure components or when computing statistical spectra. This was added in this version. This might be considered an improvement to an existing feature.

Invalid spectra appear in the Standards list.
Verify that the standards library is cleaned up whenever it is read in. This was occasionally missed.

Correlation coefficients are shown with too many decimal digits.
Correlation coefficients are altered to be shown with four rather than five decimal digits.

In Region Selection it is not possible to see the derivative of the spectrum.
Region selection did not support any of the options from the Spectra tab. Fix it so that when flag is turned on from the Diagnostic menu, then smoothing and derivative operations are honored in region selection.

The new Standards information is lost.
When standards information was created in the Standards tab, then it was possible that it might not be attached to the method until the Standards were updated. This information is saved now.

Concentrations are not saved in JCAMP-DX files.
The concentrations taken from the Standards table are not written properly into the JCAMP-DX file. All concentrations are now written.

Blank field after DATATYPE in JCAMP-DX files is not allowed.
This is a non-conformance to the JCAMP-DX paper that is found in the Foss JCAMP-DX files. It should be

supported to make things easily compatible.

The X,Y pair data format in JCAMP-DX does not work.
The implementation of X,Y pair data for JCAMP-DX did have an error that was fixed in this release. In the old implementation it resulted in an error.

Known Issues
None

TQ Analyst 8.3

- **Release date:** August 2009

New Features
SNV pathlength type allowed for Measurement Only methods.
Per customer request, the SNV pathlength type has been allowed for a Measurement Only method. Results will be reported on the SNV corrected spectrum.

Automatic conversion of spectra to Absorbance.
In an earlier version, the automatic conversion of transmittance spectra to absorbance was eliminated. A checkbox has been added to the Standards tab to allow this conversion to be made automatically for a transmittance or reflectance library and spectrum.

Implement JCAMP-DX multi-files.
If you select multiple spectra and do a Save As, then you may select to write these files to a JCAMP-DX multi-file. Also JCAMP-DX multi-files are automatically read by the Open Spectrum command and Open Standard button. If you write out a spectrum as JCAMP-DX from View Spectrum, the concentrations are written to a section of the file.

Shorten argument list for a Composite component.
A shortcut notation is supported to allow you to string many arguments in a Composite component formula. For example the new notation "2-17-3" is equivalent to "2,5,8,11,14,17" when used as the argument to a function like SDEV. The new notation is read "2 through 17 by 3. This feature is most useful for cases like "1-60-2" where it saves a lot of typing.

Resolved Issues
Unable to alphabetize classes.
Correct the problem where you attempt to alphabetize the classes when there are no standards in the method.

Crash when accessing Classes tab.
Correct the problem when standards are already defined and you enter the Classes tab with no classes yet defined.

Unexpected error if no (normal) Standards in ACLS.
Fixed a crash if you attempt to calibrate a method with no standards in the Standards tab and standards exist in the Transfer tab.

Allow more files in "Multiple Summary" menu command.
Greatly increased the buffer size to allow more spectrum names to be entered into "Multiple Summary" and "Multiple Quantify" commands.

Calibrated method opens uncalibrated.
Fixed an occasional problem where the absence of an unneeded value caused a calibrated method to appear uncalibrated.

Performance index does not appear with a classification method.
The performance index did not appear because of a conflict caused by quantitative methods. This was resolved and the value now is calculated and displayed.

In ECO software, "Quantify TQAnswers" gives no results.
An ECO software method is a special TQ Analyst method type. Make these methods behave just like the quantitative methods of TQ Analyst.

Change last character of ACLS Transfer library file name.
Changed the last character of the transfer standards file name from a tilde (~) to an underscore (_). Certain environments will not allow a file name with a tilde.

Missing component result in PLS.

Unable to read concentrations from JCAMP-DX files.
A standard with invalid data points in the analytical range for a component will cause the model for that component to be aborted. This leaves no result for that component. This is resolved by warning when an invalid data point is found.

The original JCAMP-DX paper describes an explicit format for saving concentration values into a JCAMP-DX file. Many vendors do not obey these requirements. Added features to handle most of the common non-conformances.

Unable to set maximum PCs in Discriminant Analysis.
The maximum number of principal components for all but the first class seems to be fixed at 10. Need to copy the specified value for all classes.

Known Issues
None

TQ Analyst 8.2

- **Release date:** March 2009

New Features

The new default for TQ Analyst is to not support data collection of standards.
There have been frequent problems when TQ Analyst and OMNIC are run at the same time. This is caused by a conflict between the parameter sets opened for each program. Changed TQ Analyst to default to data collection disabled.

From DDE allow the subtraction standard to be a spectrum in the current window.
Allow the ability to look for a currently displayed spectrum to be the subtraction spectrum. Do this by comparing the title of the spectrum with the title of spectra in the current display window. This is a DDE feature added for customers who have secure environments.

F-statistic as an output metric for a one class Discriminant Analysis.
Rather than an M-distance, report an F-statistic as the output metric for a one class discriminant analysis. This feature may be selected on the Other tab for Discriminant Analysis. This is a customer request.

Wavelength spectra are shown in ascending wavelength order.
Display wavelength or nm spectra in ascending order. This is a more agreeable format for NIR customers with wavelength spectra

Merge standards works on class with only one standard.
In the past the Merge Standards command button for classification methods would not produce a merged spectrum for a class with only one standard. This meant that the set of class standards might be incomplete. Now all class means are determined.

Merge Standards works with Distance Match methods.
Add the Merge Standard button to the Other tab for Distance Match methods.

Report the number of standards in each class.
Add a column in the Class table to show the number of calibration standards assigned for each class.

Move misclassified standards to the top of the Calibration table.
When there are a large number of standards in a classification method, it is very difficult to find the standards that were misclassified. They might span many pages of output. Instead move all standards misclassified by the predictor to the top of the Calibration table. This adds no new information, but it does make it far more convenient to see the standards that were misclassified.

Print a text file of the calibration information for a classification method.
When there are a very large number of standards in a classification method, it was only possible to piece together the standards information after calibration. Set up a button on the user interface that may be used to write all of the calibration information to a text file. This text file might then be imported into Excel.

Add "RMS distance from zero" as a region type.
RMS distance from zero is added as a region type for TQ Analysis methods. This is useful as a Measurement Only method for the Pfizer Variance algorithm that is used for tablet homogeneity.

Support the negative of the first derivative as a spectrum format.
For completeness add the ability to use the negative of the first derivative as a spectrum format for TQ Analyst.

Rank the outlier spectra by distance.
The Outlier diagnostic shows the extreme spectra in a calibration set. However in the output table the spectra were simply listed in their index order. It was not possible to easily see in tabular form the spectra in descending distance order. Change the diagnostic to list the spectra in descending distance order - showing the spectra most unlike the average spectrum at the top of the table.

Resolved Issues

Discriminant Analysis method opens uncalibrated.
A Discriminant Analysis method is calibrated and saved without error. However when you try to re-open it, it comes up uncalibrated.

Quantifying Raman spectra failures with mismatched spectra and method.
In some Raman TQ Analyst methods, when predicting an unknown spectrum, you get the message telling you that the spectrum and the method are not compatible. This is caused by a registration mismatch between the method and the spectrum. The spectrum is now registered to agree with the method.

Problem reading some methods with more than 100 classes.
There was a problem reading in a calibrated method with more than 100 classes.

Problems adding / deleting standards.
Problems found adding or deleting standards for special methods. The problems occurred when saving the path information or the dilution factor information.

No concentrations added to JCAMP-DX output standard spectrum.
Saving a spectrum from DDE into the JCAMP-DX format when there were no concentrations caused an error.

Possible to have Norris derivative AND Spectrum data format selected at the same time.
By switching tabs it was possible to have a method that appeared to have Norris derivative and a Spectrum data format selected. This is an impossible configuration and it was corrected on Calibration. However it should not be visible from the user interface.

Known Issues
None

TQ Analyst 8.0a

- **Release date:** June 2008

New Features
None

Resolved Issues

Cross Validation graphical results are incorrect.
The graph that is produced when you run the Cross Validation menu command shows a result with all points at zero on the x-axis. This is not consistent with the tabular data which is correct.

"Max height in range" gives an incorrect answer.
For one particular spectrum the "Max height in range" value reported in a measurement only method was incorrect. This error occurred very rarely and was caused by co-linear data points in the interpolation calculation. This also fixed a problem with quadratic baseline correction where the incorrect data value was used for the correction location.

Known Issues
None

TQ Analyst 8.0

New Features

Add support for 21 CFR Part 11 with Security Administration.
Add support for 21 CFR Part 11 by using the Thermo Security Administration software capability.

Add ability to define and use adaptive target components and standards.
Added Adaptive Target components and standards. This provides the ability to define conditional component conditions. A particular component may be computed in any of several ways depending on the unknown spectrum. Up to four target components may be specified per method. The user interface for this feature becomes visible when the "Assign target components" check box is set on the Components tab for Quantitative methods.

Add menu command the edit (change) the spectral range of the Standards library.
Add the command "Edit Standards Spectral Range…" to the Edit menu. This command will allow the limits of the Standards library to be modified. But the new limits must lie within the boundaries of the old limits.

Allow the region to be graphically edited for a SNV pathlength type.

Add the ability to use the "Edit Region" button for a SNV pathlength type in the Pathlength tab. This allows the single SNV region to be set graphically.

Up to 1000 classes are supported for classification methods.

It is possible to define as many as 1000 classes in Discriminant Analysis, Distance Match and QC Compare methods. When there are this many classes, it is best to use QC Compare.

Add ability to use a Composite component value in a Composite equation.

Add ability to include Composite component values into a Composite equation. The composite component is named with a "V" prefix. Thus the first composite component is referred to as "V1". The one limitation is that forward referencing is not allowed. That is, the result of composite component 6 may not be used in the calculation of composite component 4.

Can compute, but not report a composite component value.

It is now possible to compute, but not report a composite component value. This was done to be consistent with the feature where a composite component may be used in another composite component equation.

TRUE / FALSE results are supported in a Composite component equation.

It is possible to select the value assigned for TRUE and FALSE in a Composite Component equation. The value assigned for a TRUE and for a FALSE is assigned in edit boxes on the Composite tab.

Add FIRSTDER, SPECTRUMFIT, REGIONFIT and ACCERR as new composite component options.

Add FIRSTDER (to compute a running first derivative), SPECTRUMFIT (to report the spectrum fit metric), REGIONFIT (to report the region fit metric) and ACCERR (to report the error or uncertainty associated with the component reported by the ACCLIM composite component) as Composite components.

Add ability to read component names from a JCAMP-DX spectrum file.

The names of components may be automatically read from the CONCENTRATION field in a JCAMP-DX file when the first spectrum is added to a quantitative method from the Open button on the Standards tab. The method must have no components already defined.

Add ability to prepend to a text file that contains accumulated results.

Add a new option to how results may be added to the TQInputZ text file. Add the ability to prepend results to the file. This feature is available from the Report tab for Quantitative methods.

Copy component settings for a region to all regions with the same baseline id.

Add the ability to copy the component settings for a region to all regions with the same baseline id by clicking on the upper right corner of the Components in Region table in the Regions tab. This new feature in only supported for CLS methods.

Activate the Usage column on the calibration results display.

In the Calibration Display screen that appears when you press the Calibrate button for many techniques, there is a table that lists all of the standards that are displayed on the standards plot. The Usage column is now activated on this table. It is possible to update the Usage from this table. It is the only active column on the table. If a change is made to any usage, then the method will be uncalibrated when you exit the calibration display.

Activate the Usage column on the corrections results display.

In the Corrections Display screen (from the Corrections tab), there is a table that lists all of the standards that are displayed on the standards plot. The Usage column is now activated on this table. It is possible to update the Usage from this table. It is the only active column on the table. If the Usage change does not affect a Correction setting, then the method does not need to be recalibrated. Instead the correction is applied and an updated display is shown.

Show the class name in the PC scores diagnostic for classification methods.

For classification methods, show the class name in the PC scores diagnostic table.

Add two new "percent variance described" search types.

Add two new search types called "Percent variance described" and "Percent variance described in derivative." These are available for Search Standards and for QC Compare Search. They assume that you are searching to find a match to an unknown compound. In that case you might like to describe how much of the unknown spectrum is described by the spectrum taken from the library.

Add ability to update the null control in a quantitative analysis method.

Add ability to update the null control in a quantitative analysis method. Add a DDE command "UpdateNull" to update the correction curve information for a quantitative analysis method. This give the null adjust to work with the span adjustment provided in TQ Analyst, v.7.2. This DDE command is available in both TQ Analyst and in OMNIC.

Allow rows to be deleted from the Composite table.

Add ability to delete one or more rows from the Composite table under the Composite tab. An attempt is made to update any composite references in the composite formulas.

Resolved Issues

Calibration table for a large discriminant analysis method becomes invalid.

For a discriminant analysis method with many standards and classes, the calibration table starts correct, but becomes invalid for later standards. The cells in the table were identified with a WORD value, but if there are many rows and columns, then you need to move to a DWORD value.

Method becomes corrupt if you say No to saving changes.

If you have a quant method that is calibrated and saved, then go to the standards table and add a couple of standards. Go to File: Exit and when prompted to save changes, say no. The method becomes corrupted. (The lbd and lbt files go to zero size.) When you re-open the method, the standards are all gone. This was a problem in restoring the library after it was noted that the new method should not be changed.

Quantitative answers change if you change the default temperature and pressure values and recalibrate.

When a correction curve was generated it did not account for differences in temperature and pressure of the standard spectra. This caused incorrect correction curves and therefore incorrect predictions. The model is generated at the default temperature and pressure and then the answers are converted to the T and P for the unknown.

Improve the entry of multiple standards from the Open button on the Standards tab.

The number of files that can be opened from the Open dialog has been increased. Adding multiple standards from the Open dialog is much faster. This was accomplished by not updating the Standards table for each standard entered.

Temperature and pressure values are incorrect in the Standards table after a standard is deleted.

Incorrect temperatures and pressures were assigned when a standard was deleted. Temperature and pressure were treated as one variable and thus the temperature and pressure values were offset.

Wrong default when reprocessing an 8 cm^{-1} spectrum.

When you attempt to reprocess an 8 cm^{-1} resolution spectrum, the default comes up as 6.0 cm^{-1}. Make sure that the correct resolution comes up.

Too difficult to fill in the Components in Region table for gas analysis problems.

If the method type is CLS and there are more than eight components, then make the default entries in the Components in Region table be "not included." It is much easier to identify and fill in the specific components that will be analyzed in a region

Cannot confirm that TQ Analyst and RESULT have the same revision date for a TQ method.

RESULT reports the TQ method revision date with a date that includes the GMT offset. This was not done on the Description tab of TQ Analyst. Report the two dates identically.

Concentration data overwritten for Predict pathlength methods.

The last column of the concentration data in the Standards table was overwritten with ones when you select Predict pathlength.

Not enough precision in the values in the PC scores diagnostic tables. Too many zero values.

Show four significant digits for each PC score value. Also report the scale (exponent) of the values.

Correlation coefficient in Beer’s law method reported as zero.

In a particular Beer’s Law method the CO2 correlation coefficient calculates to zero when the units are expressed as ppm. If you express the units as %, (move the decimal 4 places to the left), the correlation coefficient calculates to 0.987. This was a scaling problem in the calculation.

Slope and intercept are not used for any other than measurement only.

As a correction for ECO products, allow slope and intercept to be used for any method type, not just measurement only.

Leverage plot gives all positive values for Studentized residual.

The leverage plot gives all positive values in the Studentized residual dimension for a Known or Predict pathlength. This occurred when all of the pathlengths were greater than one.

The correction curve doesn’t update in certain situations.

When the force thru zero option was selected, the correction curve was not automatically updated.

The ACCLIM composite component does not report an answer.
The ACCLIM composite component did not return a correct result when a subset of the components was entered.

The method file name is truncated when you print the method.
In "Print Method", the column width on the screen is used by the printer. But if the file name is longer, it gets cut off. Print the entire file name.

Incorrect number of digits printed in Multiple Summary.
In Multiple Summary, the output did not pay attention to the number of digits that are supposed to be printed.

Include file name in the Multiple Summary report.
Add the file name to the Multiple Summary report.

Multiple Quantify crashes for some methods.
Multiple Quantify has a hard crash if there are fewer Composite Components than there are regular components.

Region information is destroyed when the Sort button is used.
If there were non-consecutive baseline ids in the region table and you accessed the Sort button on the Regions tab, then the region information may be destroyed.

The uncertainty is different in TQ Analyst and QuantPad.
The algorithm for propagating the uncertainty through a polynomial correction has been changed to be compatible with the algorithm used by the QuantPad software. The Correction feature is most commonly used by gas analysis users and this gives compatibility between TQ Analyst and QuantPad.

Known Issues
None

FAQ

Why am I unable to calibrate an example method? Why am I unable to suggest regions on an example method?
If you open the tqx_pls example method it comes up uncalibrated. When you press the Calibrate button, the method does not calibrate since no regions are selected. When you go to the Regions tab, you are unable to select regions.

Example methods are saved read only. TQ Analyst does not allow you to edit any of the information on a read-only method. You need to save the method under a different name, close the method and then re-open the new method. The method will no longer be read-only and you will be able to edit the method, select regions and calibrate.

Why are some of my changes to a method forgotten when I move to another tab?
There are several places where changes must be "registered" before they are accepted. When you change

tabs and no changes have been registered, then the information in the dialog associated with the tab is not updated.

Be sure to register any changes by pressing "return" or tabbing to the next field on the dialog.

Why am I unable to edit a method that I copied from a CD-ROM?

If you copy a TQ Analyst method from a CD-ROM onto your system disk, the method cannot be edited.

When you copy a method from a CD-ROM, the files that make up the method are written read-only. TQ Analyst does not allow you to edit any of the information on a read-only method. You need to save the method under a different name, close the method and then re-open the new method. The method will no longer be read-only and you will be able to edit the method, select regions and calibrate. An alternative is to go into the Properties of the TQ Analyst method files and turn off the read-only selection.

TQ Analyst 7.2

New Features

The EMEA Maximum Wavenumber Distance algorithm is supported.

The EMEA standard describes the use of a Maximum Wavenumber Distance (MWD) algorithm. This is the second, tie-breaking metric computed by the normal Distance Match algorithm. It is now possible to rank the classes according to the MWD criterion by checking that option on the Other tab when the Distance Match technique is selected.

TQ Analyst methods may now use more than 1700 standards.

In all versions of TQ Analyst up to and including 7.1, the maximum number of standards that could be added to a single method was ~1700. This limit has been relaxed in 7.2 where many more standards. There remain a maximum number of standards that may be supported, but this number is approximately 32,000. The major impact of this change is in all TQ Analyst tables that show standards. When this change is made, each standards table is not shown in its entirety. Only portions of the table are displayed. The table entries that are shown are updated based upon the currently selected standard.

TQ Analyst supports cross-corrections as done in QuantPad.

QuantPad includes a features which allows a post-correction of component amounts using equations that include terms using the amount of other components. This same feature is now supported in TQ Analyst. The feature is available from the Corrections tab.

Add ability to reset the measurement temperature and pressure for a quantitative analysis method.

Add a DDE command "UpdateMeasurementTP" to update the default temperature and pressure assigned for all incoming samples. This matches a feature in QuantPad. This DDE command is available in both TQ Analyst and in OMNIC.

Add ability to update the span control in a quantitative analysis method.

Add a DDE command "UpdateSpan" to update the correction curve information for a quantitative analysis method. This give the span adjust that is necessary to be compatible with QuantPad. This DDE command is available in both TQ Analyst and in OMNIC.

Component concentrations added to the Principal Component Scores diagnostic.

The Principal Component Scores diagnostic is used to view the pairwise interaction between the scores for each standard associated with a method. For quantitative methods, this change adds the ability to view if there are any interactions between any of the pc scores and the component amounts.

Make the Principal Component Scores diagnostic available for CLS and QC Compare Search techniques.

Allow the Principal Component Scores diagnostic for Classical Least Squares (CLS) and QC Compare Search techniques.

Only display the outermost 100 standards in the Spectrum Outlier diagnostic.

The plot that accompanies the Spectrum Outlier diagnostic shows the distribution of distances from the center of the standards. As the number of standards becomes large, viewing the entire set of standards is less informative. Since we only care about the extreme values, only display the 100 standards that have the largest distance from the center of the distribution. This set contains all of the information about outlier spectra.

Ability to quantify a csv spectrum is added.

Add the ability to quantify a properly configured csv (comma separated variable) spectrum file. The file must be compatible with the TQ Analyst method and it must be saved with one data point (x, y pair) per line.

The Index column matches the standard number from the Standards tab.

The index column in many of the diagnostics displays now displays the same number as the standard in the Standards tab. This makes it easier to match up standards between the Standards tab and the diagnostic. In the past the Index column simply incremented per row in the table.

Added two new region types to the Region tab

Two region types have been added:

Region Type	Description
Location of max height in range	the (interpolated) x axis value at which the maximum y-value is found
Location of min height in range	the (interpolated) x axis value at which the minimum y-value is found

"Location at % of peak maximum" replaces four region types.

There are four peak region types of the form "Location at <n>% of peak maximum" where <n> is 1, 2, 5 or 10. These are a special case of the new region type "Location at % of peak maximum." The four old types are no longer available. When an old method is read into TQ Analyst, these regions are automatically converted. An old method may still be used to predict an unknown spectrum.

Support the fast 0.5 cm^{-1} collect for Reprocess.

A "fast" 0.5 cm^{-1} data collection is supported by RESULT IGS software. The ability to reprocess with these collection parameters is added to the Reprocess Command.

Add "Range" to output from "External Validation" and "Quantify Multiple."

The range for each component over all samples measured is added as a statistic available from the "External Validation" and "Quantify Multiple" commands. This information is only available from the `[TQDiag SlopeAndIntercept]` DDE parameter.

Allow the subtraction spectrum in the \Spectra directory.

For a Measurement Only method it is important that it be possible to save the subtraction spectrum into a directory that can be written. The best candidate is the \Spectra directory where a collected spectrum is normally saved. For a Measurement Only method, the subtraction spectrum may be either in the same directory as the method or it may be in the \Spectra directory

Automatically read concentration values from a JCAMP-DX spectrum.

When a JCAMP-DX spectrum is read into the Standards table, the concentrations are automatically extracted from the CONCENTRATIONS line in the JCAMP-DX spectrum.

Read concentrations written in exponential form from the spectrum comment.

When a .SPA file is read into the Standards table the concentration values will be taken from the spectrum comment. These concentration values may now be entered in exponential form.

"Baseline Scale" added to View menu.

A new display format is available. Using this format, all spectra in the spectral display window are scaled so that their lowest baseline point is at the extreme of the display and the amplitude of each spectrum is common for all of the spectra. This is available to replace doing a Full Scale, followed by a Common Scale, followed by dragging all of the spectra to share the same baseline.

Add "Range" and "Count" as Composite component functions.

The keywords "RANGE" and "COUNT" are available from the Composite component tab. The range term is the difference between the maximum value and the minimum value in the set of arguments to the function. The count term is the number of entries in the argument list.

Add "Correlation Coefficient", "Slope" and "Intercept" as Composite component functions.

The keywords "CORCOEF", "SLOPE", "INTERCEPT" and "ZSLOPE" are available from the Composite component tab. Each of these functions assume that the list of arguments are passed in the form (x1,y1,x2,y2,x3,y3,…). Then the correlation coefficient is the correlation between the list of `x` values and the list of `y` values. The slope, `m`, and intercept, `b`, are the results of `yi = m xi + b`. The ZSLOPE composite component reports the slope when the intercept is forced to zero. That means that the model is `yi = m xi`.

Composite component arguments may be enclosed in brackets.

In addition to be able to enclose composite component arguments in parentheses, the arguments may also be enclosed in brackets ([and]).

More composite components may be read from text files.

Composite components, or entries in the composite component argument list, may be read from a text file.

Entries from Y1 to Y999 may be used, The Y entries are found in file tqinputy.txt. Entries from Z1 to Z999 may also be used. These entries are found in file tqinputz.txt.

Text files used by Composite components may be found in the temp directory.

If the text file required by Composite components is not found in the same directory as the method, then it may be located in the user's temp directory.

Define the decimal and item separators for Composite components.

Edit boxes are available in the Composites tab to define the decimal and item (list) separators that are used in the composite formulas.

Add operator to report the absolute value of the difference Composite components.

The underscore character (_) is used as an operator to denote the absolute value of the difference between two numbers. Thus `3.5 _ 4.7` equals +1.2. This operator is useful for some instrument diagnostics.

TQ Analyst answers may be written to or appended to a text file.

Three check boxes are available in the Results section of the Report tab. These selections allow the results of each quantify to be written to a text file, to be appended to a text file or clear the text file. The text file is tqinputz.txt and it is located in the user's temp directory. A DDE command, `DeleteQuantAnswerTextFile`, is present to clear the text file.

Put the results reported by TQ Analyst into a DDE parameter.

The variable `[Quantify TQAnswers]` contains the results from the most recent prediction of an unknown spectrum. The component name may be found by using the DDE command `GetComponentName`. If the method is a classification method, then the associated class names may be found by using the DDE command `GetClassName`.

Spectra tab is always present.

The Spectra tab is now always visible for a TQ Analyst method. It no longer must be turned on from the Measurement or Standards tab.

Add "Use Processed Spectra for Diagnostics" menu item.

This menu item is now found at the top of the Diagnostics menu. It defines whether diagnostics are performed based on the standard spectra or based on the results of the operations in the Spectra tab on the standard spectra.

The Usage column is fixed when rotating through components.

The Usage column in the Standards table is now frozen when we loop through all of the component concentrations. This allows this field to be viewed as concentrations are entered.

DDE Commands are available to get the Component Names or the Class Names.

DDE commands `GetComponentName` and `GetClassName` are available to report a component name or a class name in the method. The first argument is the (one-based) number of the component or class to be reported. Any composite components may also be reported. The result is returned in `Quantify TQNames`. If a second argument of "U" is used, then the returned value is the unit for the component number. If a second argument of "A" is used, then the returned value is the component / class abbreviation.

Add the second best result to Multiple Summary.
If there is more than one category in a Discriminant Analysis, QC Compare Search or Distance Match method, then the second best class result is added to the Multiple Summary report.

Remember the sort order for Standards after changing tabs.
Standards may be reordered on the Standards tab based on alphabetical or numerical order. However this order was not maintained when you switched to a different tab and then returned to the Standards tab. The sort order is now remembered when you switch to a different tab. Upon reentering the Standards tab, the sort order is the same as when you left the tab.

Resolved Issues

Correction for temperature and pressure is done incorrectly.
The gas law correction for temperature and pressure is done backwards.

The backspace key doesn’t work.
The backspace key does not work properly in the tables, edit boxes and dialogs that are part of TQ Analyst.

A Mem Pointer error occurs when exiting TQ Analyst.
When the TQ Analyst program is terminated on some systems, there is a Mem Pointer error dialog that appears. This occurs only when an international character set is installed on the system.

Error when attempting to do SNV after smoothing the spectrum.
If you attempt to perform SNV after smoothing the spectrum or taking the derivative of the spectrum, then the result was not correct.

Temperature and pressure values are reset to default.
This problem occurs when a method is set up to require temperature and pressure for each standard. When a new standard (or standards) is added to the method and the method recalibrated, the temperature and pressure values return to their default values.

Pressure values incorrect when QuantPad method loaded into TQ Analyst.
The pressure values from QuantPad are entered into the Standards table in units of hPa, not torr.

ValPro Algorithm Verification fails in French and German.
A composite component test fails. It is the test using data from a text file. The error is caused by the different decimal separator. The text file has a period for its decimal separator and this causes the value to be read improperly from the file.

Adding a region causes TQ Analyst to crash.
This problem occurs when the number of regions exceeds the number of components.

Can’t predict a spectrum because of a region mismatch.
If one of the TQ Analyst regions is very close to the endpoint of the spectrum, then there could be a situation where rounding causes the region endpoint to look to be outside the limits of the spectrum.

The number of factors used in PCR is updated when it shouldn’t be.

In PCR setting the number of factors to use for prediction should not occur automatically. It is the user’s responsibility to set this value. However it was being done automatically based on when the best set of results was found.

Percent variance is reported incorrectly after PCR calibration.

The percent variance value that appears on the calibration results dialog for a calibrated PCR method gives an incorrect value. Sometimes it may be incorrect by orders of magnitude.

Error saving a list of classes in RESULT and predicting with TQ Analyst.

In a RESULT workflow it is possible to loop through and save a set of class names. Then in a second, usually automatic, loop you can collect spectra. The problem is that the class names and the measurements from the collected spectra could not be correlated.

The Standards to Text File command fails if there are more than 500 standards.

If you attempt to write the standard spectra into a text file with the "Standards to Text File" menu command, the operation will fail if there are 500 standards. In the corrected version the write will still fail, but not until there are many more standards.

Error in values reported by the Principal Component Scores diagnostic.

If mean centering and variance scaling are applied to the data, then it was applied for a second time before performing the principal scores diagnostic. This caused the values that are displayed to be incorrect.

Incorrect standard selected in Spectrum Outlier diagnostic for an ACLS method.

If you performed the spectrum outlier diagnostic on an ACLS method and selected one of the transfer standards, then you would not be shown the correct information.

Pressure reported by Composite Component is incorrect.

When the XP parameter is specified as a composite component, the reported value is incorrect. The pressure value is being treated as if it were in hPa unit. However the conversion to torr has already taken place.

Incorrect values reported for "Peak width (low loc referenced)" and "Peak width (high loc referenced)."

Region types "Peak width (low loc referenced)" and "Peak width (high loc referenced)" gave erroneous results. This is a very specialized region type and has been little used.

Transfer calibration standards are not included in mean centering or variance scaling.

Mean centering and variance scaling did not include the contributions from transfer standards. While this is an acceptable assumption, it is better to include these in the calculations.

After quantifying, the DDE variable "Result Array" contains values that shouldn’t be reported.

"Result Array" should show only the components (and composite components) that are supposed to be displayed in a report. Instead all of the components are shown.

Calibration is not always the same for a CLS method.

There are times when the calibration of a CLS method is not correct. This is most likely to happen after some PLS methods have been calibrated beforehand. The problem is that the variance scaling value is not initialized properly.

There will be situations where an old, calibrated method will become uncalibrated by this fix.

What does it mean for the components in a PLS method to "Always sum to a constant" when there is missing data in the concentration information?

It is possible to have a PLS method set up to "Always sum to a constant" and at the same time have missing data values in the concentrations on the Standards tab. This is inconsistent.

Multiple Quantify shows dates instead of numeric results.

If you run the Multiple Quantify menu command in a language that uses the decimal point as anything but the decimal separator, then the numeric results in the summary report look like date strings.

I didn’t change anything, but the method became uncalibrated when I left the component tab.

If you change a value in a calibrated method and then return the value to its original state on the Components tab, then the method will become uncalibrated.

Spectrum and method mismatch on a method with a subtraction spectrum.

The subtraction spectrum can cause a method to mismatch with a spectrum that is to be measured. A slight shift of the spectral region can cause this.

The Usage symbol is incorrect for transfer standards on the Calibration graphs.

When you calibrate an ACLS method, the calibration display does not assign the correct symbol to the transfer standards. You cannot tell that a transfer standard is a calibration standard by looking at the symbol on the graph.

The RMSECV value in Cross Validation is incorrect for a Known pathlength method.

If you run the Cross Validation diagnostic on a method where the pathlength type is set to Known, then the RMSECV value is incorrect. Also the entries in the Cumulative PI and Component PI columns of the table are incorrect.

Crash when quantifying a spectrum with different spectral range than TQ Analyst method.

If you attempt to quantify a spectrum which has a spectral range that is larger than the spectral range of the standards in the method, the prediction step may be abnormally terminated and the application must be restarted.

Similarity Match warning value is not saved properly.

For a Similarity Match method, if you change the state of the "Match value check" check box and then save and close the method, the new value will not be shown when the method is reopened.

Known Issues

None

FAQ

Why am I unable to calibrate an example method? Why am I unable to suggest regions on an example method?

If you open the tqx_pls example method it comes up uncalibrated. When you press the Calibrate button, the method does not calibrate since no regions are selected. When you go to the Regions tab, you are unable to select regions.

Example methods are saved read only. TQ Analyst does not allow you to edit any of the information on a read-only method. You need to save the method under a different name, close the method and then re-open the new method. The method will no longer be read-only and you will be able to edit the method, select regions and calibrate.

Why are some of my changes to a method forgotten when I move to another tab?

There are several places where changes must be "registered" before they are accepted. When you change tabs and no changes have been registered, then the information in the dialog associated with the tab is not updated.

Be sure to register any changes by pressing "return" or tabbing to the next field on the dialog.

Why am I unable to edit a method that I copied from a CD-ROM?

If you copy a TQ Analyst method from a CD-ROM onto your system disk, the method cannot be edited.

When you copy a method from a CD-ROM, the files that make up the method are written read-only. TQ Analyst does not allow you to edit any of the information on a read-only method. You need to save the method under a different name, close the method and then re-open the new method. The method will no longer be read-only and you will be able to edit the method, select regions and calibrate. An alternative is to go into the Properties of the TQ Analyst method files and turn off the read-only selection.

TQ Analyst 7.1

New Features

6.0 cm^{-1} data collect for standards is supported.

The 6.0 cm^{-1} data collect of standards is now allowed. If OMNIC_ra.dll is installed and indicated in the registry, then it is possible for the Raman collect to be indicated in Experiment Setup. However if the instrument is an Almega, then it is not possible to collect standards from TQ Analyst.

Numbers in composite component formula may include an exponent.

The numbers in a composite component formula may now include an exponent. The forms of a number with an exponent that are allowed include 1.234e4, 1.234e+7 and 1.234e-5. The lower case "e" denotes an exponent.

Strings in the Standards table will be sorted into the same order as Excel.

The Sort button on the Standard tab has been changed when applied to text strings. The change makes the sort order the same as the sort order found in Excel. The different order is primarily reflected in the File Title column. In Excel purely numeric values are sorted before numeric values that are the leading characters in a longer string.

A Mahalanobis distance from zero may be computed and reported.

If Discriminant Analysis is done with one class, then the mean centering check box determines if the class mean is removed from the class before computing the Mahalanobis distance. If the mean centering box is not checked, then the M-distance from zero is computed. Whenever more than one class is available, then the class mean is always removed.

A Correlation Coefficient command is added to the View menu.

A "Correlation Coefficient" command is added to the View menu. The command is inactive unless there are two spectra selected in the current window. The result is shown in a message box. The coefficient is computed from the region selected in the spectral window. Three correlation coefficient values are shown. The first is the r value when each spectrum has its mean value removed. The second is the r value when the first difference of each spectrum is taken before the value is computed. The third is the r value for the uncorrected spectrum.

A New Window command is added to the Window menu.

A "New Window…" command is added to the Window menu. This will open a new, empty spectral window.

A new region type to report the Euclidean distance between a spectrum and zero is available.

A new region type, "Euclidean distance from zero" has been added on the Regions tab. This measurement is most useful with derivative spectra on spectra measured from array automation, but it can be used with any spectrum type.

The SNV pathlength correction may be done before or after a derivative or smoothing is performed.

If you select the SNV pathlength type and perform a derivative on the data or smooth the data, then the pathlength correction was always done before the derivative or smooth. If you were able to switch the order of these operations, then you’d get a slightly different result. This option is now present on the Spectra tab. The option is only available when the SNV pathlength option is selected.

The ability to change the Class for multiple standards at one time has been added.

The class assigned for multiple standards may be changed simultaneously from the Standards tab. This will be done by selecting the Class label which calls up a dialog box from which you may identify the new class value (number) and the standards that will be assigned to that class.

Special codes have been added to automatically convert units in the Standards tab.

Several special codes have been added to the values entered in the Standards tab. The special codes provide an automatic conversion between units. The conversion is performed when you leave the Standards tab. When you return to the Standards tab, the new, converted value will be visible.

Regions may be sorted by frequency and baseline ID.

A "Sort Regions" button has been added to the Regions tab. This button is active for all methods except for Simple Beer's Law and SMLR. The spectral regions are sorted numerically. If the method type is CLS, then the list of regions is also sorted so that regions that share the same baseline region (Baseline ID) are listed consecutively.

Standard error or uncertainty value is available as a Composite Component.

The keywords "ERROR" and "UNCERT" are available from the Composite component tab. When more than one component is specified as an argument, then the largest error (or uncertainty) term is reported.

Resolved Issues

Variance scaling for Discriminant Analysis not available.

The Variance scaling option on the Other tab for Discriminant Analysis was not active.

Within class variance reset when switching between Distance Match and Discriminant Analysis.

When a Discriminant Analysis method was switched to Distance Match and then returned to Discriminant Analysis, the status of the Within Class Variance check box on the Other tab was reset.

The frequency range when opening a third party spectrum does not match the spectrum range in the third party software. The frequency ranges are vastly different.

When a spectrum with a "laser frequency" different from 15798.0 cm^{-1} is brought in to TQ Analyst, it is normalized to the theoretical HeNe laser frequency. If the difference in laser frequency is small (<~16 cm^{-1}), then the there is no problem. However if the laser frequency difference is large, then the new spectrum has a shifted frequency range and is not a good representation of the original spectrum. This is especially useful when the data spacing is an exact number like 4.0 cm^{-1} or 12.0 cm^{-1}.

Unable to read an old measure only method.

In some old methods, the target peak location for a measure only method may be set to some small, but non-zero number. This caused an error reading the method.

Unable to determine is an outlier is rejected because of the Dixon test or the Chauvenet criterion.

If outliers are detected from the "Spectrum Outlier…" command, a message is needed to indicate if the outliers are a result of the Dixon test or the Chauvenet criterion.

AddStandardToMethod command does not handle the pathlength for a Known pathlength method.

When you use the `AddStandardToMethod` DDE command to add the first standard to a Known pathlength method, the pathlength value passed as an argument is ignored. In the Standards table the pathlength is set to zero.

Component in Region information is inaccurate after deleting a component.

If you delete a component or components from a quantitative method, then the component in region information as shown in the Regions tab is not accurate. The new component in region information is

transposed.

The standard error is being reported as zero and that does not seem to be possible.

In gas analysis it is possible to have small analysis regions combined with many components and interferences. In this case the number of degrees of freedom for the measurement standard error may dip below zero.

The percent difference display in the Edit Corrections window in distorted when there are zero concentration standards.

In the Edit Corrections window, the right display shows the percent difference between the corrected and actual value. Especially in gas analysis there are frequently zero concentration values. This may cause the y axis scale of the display to be grossly distorted, hiding the changes for values greater than zero.

The line drawn for the corrections curve in Edit Corrections may not be updated properly.

In the Edit Corrections window, the line drawn on the display may not update properly. This occurred after the "Save Changes" button was pressed.

Pathlength composite component is incorrect for a Known pathlength method.

If the pathlength type is set to Known Pathlength, and an unknown spectrum is quantified, the pathlength value returned as a composite component is incorrect. The pathlength was not set into the proper parameter.

Standard errors reported are larger than errors from QuantPad.

The standard errors reported for gas analyses from CLS methods are considerably larger than the standard error values reported by QuantPad.

Crash when accessing the Edit Corrections function.

There is an occasional hard crash of the software when the Edit Corrections button is pressed from the Corrections tab. The software must be restarted to continue.

Crash when accessing the Regions tab with a gas analysis method.

When using a gas analysis method with many components and regions, there are situations when the Regions tab locks up and the program will not continue. The software must be restarted to continue.

Known Issues

The backspace key doesn’t work.

The backspace key no longer functions properly in the tables, edit boxes and dialogs that are part of TQ Analyst.

A Mem Pointer error occurs when exiting TQ Analyst.

When the TQ Analyst program is terminated on some systems, there is a Mem Pointer error dialog that appears. It does not appear to harm anything, but it is annoying.

FAQ

Why am I unable to calibrate an example method? Why am I unable to suggest regions on an example method?

If you open the tqx_pls example method it comes up uncalibrated. When you press the Calibrate button, the method does not calibrate since no regions are selected. When you go to the Regions tab, you are unable to select regions.

Example methods are saved read only. TQ Analyst does not allow you to edit any of the information on a read-only method. You need to save the method under a different name, close the method and then re-open the new method. The method will no longer be read-only and you will be able to edit the method, select regions and calibrate.

Why are some of my changes to a method forgotten when I move to another tab?

There are several places where changes must be "registered" before they are accepted. When you change tabs and no changes have been registered, then the information in the dialog associated with the tab is not updated.

Be sure to register any changes by pressing "return" or tabbing to the next field on the dialog.

Why am I unable to edit a method that I copied from a CD-ROM?

If you copy a TQ Analyst method from a CD-ROM onto your system disk, the method cannot be edited.

When you copy a method from a CD-ROM, the files that make up the method are written read-only. TQ Analyst does not allow you to edit any of the information on a read-only method. You need to save the method under a different name, close the method and then re-open the new method. The method will no longer be read-only and you will be able to edit the method, select regions and calibrate. An alternative is to go into the Properties of the TQ Analyst method files and turn off the read-only selection.

TQ Analyst 7.0

New Features

QuantPad methods can be opened using the open command in the file menu.

The method will automatically be converted into TQ Analyst form. You may automatically open the reference standard spectra by identifying the path where the standards are found. Regardless of the status of the QuantPad method, the converted method will open "uncalibrated".

The Default Method Path command was added to the file menu.

This command brings up a dialog from which you can define a new starting path for TQ Analyst method file operations. This defines the starting directory that will open when you use the Open Method, Save Method and Save Method As commands.

The Default Spectrum Path command was added to the file menu.

This command brings up a dialog from which you can define a new starting path for spectral file operations. This defines the starting directory that will open when you use the Open Spectrum and Save Spectrum As commands.

The Process Selected Spectra command was added to the view menu.

This command takes the spectrum or spectra in the current display window and applies the corrections indicated on the Spectra tab to the spectrum or spectra. If only one spectrum is selected, then the resulting spectrum is shown in the same display window. If more than one spectrum is selected, then the resulting spectra are shown in a new window. If the spectrum or spectra have already been processed, then no action is taken.

The Multiple Summary command was added to the Diagnostics menu.

Like multiple quantify, this command takes multiple .spa or .spg files and produces a summary report of the predicted results on all of the spectra. The multiple summary command produces a table where each row details the measurements for a single sample spectrum.

The Quantify Sequence or Map command was added to the Diagnostics menu.

This command is grayed unless the QuantSequence.exe program is available. This program is installed with the RESULT sequence add-in of RESULT software and may be installed with other Thermo Scientific products. If the program is available, then a sequence file (with extension .srs or extension .map) may be selected and a new concentration file (.cnc extension) will be created.

The Loading Spectra command in the Diagnostics menu produces a result for a Discriminant Analysis method.

A set of loading spectra for each class may be viewed for a discriminant analysis method.

Ignore Zeros option was added to the Calibration Results window of Quantification Methods.

When this option is checked, the y axis limits of the difference display (the right side display) are computed ignoring any zero x axis concentrations. This is especially important for gas analysis where pure component (or few component) standards are used frequently.

The Pathlength tab is now available for Search standard and QC Compare methods.

There are four pathlength options. They are Constant, Peak ratio or Normalize, Multiplicative signal correction and Standard normal variate

Added new options for Known pathlength

These options include:

- Ability to determine pathlength from a pathlength region when samples are quantified
- Ability to define the pathlength region that will be used when samples are quantified
- Ability to apply a slope and intercept to the pathlength measurement before it is used to normalize the result

Added Pathlength correct option for Known, Internal Reference and Peak Ratio or Normalize pathlength types

Add the ability to apply a slope and intercept to the pathlength measurement before it is used to normalize the result

Dilutions and Extractions feature moved to Advanced button of Pathlength Tab

The dilutions and extraction options were located on the pathlength tab, now they are available by pressing the Advanced button on the Pathlength tab.

Added a Gas Law Corrections feature to Advanced button of Pathlength Tab

This feature allows the method developer to model temperature and pressure in the quantitative method.

Added an Alphabetize button to the classes tab

The Alphabetize button permanently reorders the class names into alphabetical order.

Added Use threshold limits option to Components tab

When this option is selected the method can be configured to report all measurement results outside of the limit, as either the limit value or a NaN value.

Added Allow composite components option to Components tab

Allows the definition of a new type of component that is computed from the results of components on the components tab.

Added Result Column to Components table of Components tab

Provides numerous options for controlling the output of measurement results. This option is settable per component. New settings for this option include:

- Compute and report as zero if negative
- Compute as zero if negative (do not report the result)
- Compute and report as zero if < error
- Compute as zero if < error (do not report the result)
- Compute & report as limit if outside of acceptance
- Compute as limit if outside of acceptance (do not report the result)
- Report as threshold limit if outside threshold
- Report as undefined if outside threshold

Added Use threshold limits option to Measurements tab

When this option is selected the method can be configured to report all measurement results outside of the limit, as either be reported as the limit value or a NaN value.

Added Allow composite components option to Measurements tab

Allows the definition of a new type of component that is computed from the results of components on the components tab.

Added Result column to Measurements table of Measurements tab

Provides options for controlling the output of measurement results. This option is settable per component. The settings for this option include:

- Compute and report
- Report only
- Report as threshold limit if outside threshold
- Report as undefined if outside threshold

Added Use special format option to Measurements tab

When interferograms are saved with the final format spectra, measurements can be performed on any of the following spectra:

- The final format spectrum
- The single beam of the sample spectrum
- The interferogram of the sample spectrum
- The single beam of the background spectrum
- The interferogram of the background spectrum

Added Composite Components tab

Allows the definition of components that are computed from the results of components on the components tab.

- Supports an algebraic equation to be defined for each of the composite components
- Multiplication by constant values supported
- Addition, subtraction, multiplication and division of component values supported
- Unlimited usage of parentheses supported
- Supports special functions to be used to combine results
- Sum of component values
- Average of component values
- Standard deviation of component values
- Maximum of component values
- Minimum of component values
- Maximum of the absolute value of component values
- Minimum of the absolute value of component values
- Allow pathlength, temperature or pressure to be reported

Added Restrict y-axis range in sample spectra option to Standards tab

If this option is selected and the method type is QC Compare Search or Search Standards, then any data point that fails the y-axis cutoff is ignored in computing the search metric. When this option is selected for any other method type, the intensity of any data point that fails the y-axis cutoff is reset to the limit value.

Added Missing Data option to Standards tab

The method developer may define a specific concentration value to indicate a missing concentration value. TQ Analyst uses -100 by default. When a PLS method is calibrated with standards that have missing values, the standard will be used to develop calibration models for components will real measured values and will be ignored for components with missing values. For all other quantitative method types, the standard is included in the calibration.

Added ability to change the Usage of multiple standards

When you click on the Usage header on the standards table a dialog will appear allowing you to specify the new usage and a set of standards. The possible inputs for the usage are Calibration (CA), Validation (VA), Correction (CO) or Ignore (IG). You are allowed to list which standards will take this new Usage value. Possible entries include the following

ALL

1,3,5,7

1-100

1,5-8,11-14,17

Added Temperature and Pressure values for Gas Law Corrections to Standards tab

Temperature and Pressure values can be recorded in the standards table if Gas Law Corrections are specified using the Advanced button of the Pathlength tab.

Added Allow spectral processing option to the Standards tab for Search Standards and QC Compare Search methods

In prior versions of TQ Analyst, Search Standards and QC Compare Search methods didn’t support spectral processing.

Added Show processed spectra in View Standards option to the Standards tab for Search Standards and QC Compare Search Methods

In prior versions of TQ Analyst, Search Standards and QC Compare Search methods didn’t support spectral processing.

Added Apply spectral processing to the standard spectra option to Spectra tab

Check this option if you want to apply spectral processing to both the standards and the sample spectra. Uncheck this option of the spectral processing is being applied to the sample spectra in order to match the spectral processing performed on the standards before they were added to the method.

Added Apply spectral processing to the pathlength region option to Spectra tab

This option allows you to control whether spectral processing will be performed on the pathlength region. This option is only available for methods that use a pathlength treatment that requires a pathlength region.

Added Spectral subtraction option to the Spectra tab

This option permits you to subtract a spectrum from each unknown and perhaps standard spectrum that is used in the method. The point-by-point spectral subtraction will take place before any other action is applied to the unknown or standard spectrum. The subtraction spectrum must have the same name as the TQ Analyst method and be found in the same directory as the method.

Added new region types to the Region tab

The following region types have been added:

- Peak width (at % of maximum)
- width measured at a certain % of the peak maximum (read from % or Ht column)
- Peak area (within % of maximum)
- peak area measured between the limits of a certain % of the peak maximum (read from % or Ht column)
- Peak width (low loc referenced)
- set the low frequency location of the peak width, seek the high frequency location at the same intensity and determine the width
- Peak width (high loc referenced)
- set the high frequency location of the peak width, seek the low frequency location at the same intensity and determine the width
- COG peak location (% threshold)
- report the center of gravity (COG) peak location where the COG is computed from a certain % of the height (read from the % or Ht column).
- Location at % of peak maximum
- find the peak maximum and then determine the location where the intensity is at a % of the maximum (read from the % or Ht column).
- this is the generalization of the "Location at 10% of peak maximum" region type
- Location to match Ht (low loc referenced)
- start at the low location (frequency) region limit and determine the first location where the y-axis Height is found (target height read from the % or Ht column).
- Location to match Ht (high loc referenced)
- start at the high location (frequency) region limit and determine the first location where the y-axis Height is found (target height read from the % or Ht column).

Added the ability to copy the contents of one row to another in the Components in Region table of the Regions Tab

Region tab \ Components in Regions table \ Numbered row of table

When you select a number in the first column of the table, it is possible to indicate that you want to set the entries to be identical to the previous row of the table. A dialog appears to give you this option.

Added the ability to copy the contents of one row to many other rows in the Components in Region table of the Regions Tab

Region tab \ Components in Regions table \ Index label

When you select the Index header on the table, you may define a row that will be copied. Then in a second entry, you can define all of the rows that will match the selected row. If the method is CLS and the region type is "Linear removed", then the Baseline ID column in the Regions table is also copied.

Added support for component interferences to the Components in Region Table of the Regions Tab for CLS Methods only

For CLS Methods, each entry in the Components in Regions table is a drop down with the following selections

- - - the component does not contribute in this region
- + - the component does contribute in this region and should be used to determine the component
- intf - the component contributes in this region, but it is an interference and should not be used to determine the component

Added Always use one-at-a-time cross validation option to Other Tab for PLS methods only

This option allows the user to set up the full calibration step to cross validate by removing one standard at a time. In the normal situation, when there are a large number of standards multiple standards are removed during each cross validation step.

Added the ability to identify correction standards that will be used for only one component

By selecting "Correct with non-zero correction standards only" you can selectively identify a correction standard for one component only. The concentration of all other components must be zero which causes the correction standards to be ignored for the other components. If you want to use any of the calibration standards as part of the correction curve, then you need to include them with zeroes for all other components. This provides capability that is equivalent to a feature found in QuantPad.

Added Galactic type correlation search to the search type option list on the Other Tab for Search Standards methods and QC Compare Search Methods

This search type computes a correlation value using the correlation algorithm supported by Galactic software. Rather than doing the correlation on a first difference spectrum, the Galactic algorithm, mean centers the spectrum and computes the correlation on the corrected spectrum.

Added Enhance correlation metric to the Other Tab for QC Compare Methods

The QC Compare method has always used an algorithm to spread out values that are close to 100 (a perfect match). This is a monotonic function relative to the normal search metric. This option allows you to report the same metric that is reported by Search standards. This metric has less discriminating power when the match is close to 100. The order of the best hits is identical for the two algorithms.

Added Pass/Fail indicator option to Report Tab for Quantitative and Measurement methods.

This option was available for qualitative methods in prior versions of TQ Analyst. Now it is supported for all method types.

Resolved Issues

The date on the lbd and lbt files changes for a QC Compare method when I quantify an unknown spectrum.

If there are standard spectra set to "Ignore" in your method, then these spectra temporarily get set to deleted in the library when you predict an unknown. This causes the library to be rewritten.

Intercept is set to Nonzero, but the printout says Zero.
If you print out a Simple Beer's Law method where the intercept for a component is set to nonzero, then the report will indicate a zero intercept.

TQ Analyst crashes if the user is not an administrator.
TQ Analyst crashes if the user is not logged on as an administrator.

No warning given when changing a signed TQ Analyst method.
Open a signed TQ Analyst method, add standards and change the method type. There is no warning that a signed method was changed. Also there is no warning when the saved method is saved.

Cannot add to the middle of a Standards table.
It is not possible to add standard spectra into the middle of a Standards table.

Standard normal variate (SNV) pathlength results are incorrect in some cases.
If you select SNV pathlength and either smooth or take the derivative of the spectral data, then the calibration results are incorrect. There are other cases where SNV pathlength correction gives incorrect results.

Known Issues

The region information is lost when you switch to a PLS or PCR method type
If you switch from a method that has peak height, area or width region information to a PLS or PCR method, the region information is lost without warning.

The workaround for this problem is to store the method to a new, temporary name before switching among the method types.

The axes on the Calibration display are misleading
Upon calibrating a method, the x- and y-axis values that appear in the calibration window are misleading. For instance the labels for the X axis may be -0 and 3 when, in reality, those numbers should be -0.2 and 3.2.

Since there are not enough digits displayed on the graph, view the values in the table after you select a standard.

Sorted columns don't stay sorted
When using the Sort command on the Standards tab, the sort order if the user tabs away from the standards page and comes back.

FAQ

Why are some of my changes to a method forgotten when I move to another tab?
There are several places where changes must be "registered" before they are accepted. When you change tabs and no changes have been registered, then the information in the dialog associated with the tab is not updated.

Be sure to register any changes by pressing "return" or tabbing to the next field on the

dialog.

Why does the incorrect data appear in Excel when I perform a Multiple Quantify, Multiple Summary or External Validation command?

If the Excel spreadsheet for the previous instance of a command is still open, then the old data appears is shown. The spreadsheet does not update and is not overwritten.

Make sure that Excel is not open when you run these commands.

Why does the font change in the tab displays while I'm running TQ Analyst?

The cause for this is not known.

TQ Analyst 6.2a

New Features

New column added to the Calibration Result Table for Distance Match and Discriminant Analysis.

There is a new column in the calibration result table for distance match and discriminant analysis methods. The column, which is unlabeled, lies between the Actual Class column and the Calculated Class column. There is an entry in this column only when the calibration model misclassifies the standard spectrum.

A new warning may be reported with all classification methods. The warning indicates that the calculated class does not match a specified class.

There is a new entry, Class check, in the Report tab for all classification methods. You can select a specific class that is the expected answer. If the class that is calculated from the model does not match this class, then a warning is issued.

Resolved Issues

There may be errors in the usage column of the Standards table when more than one class is deleted from a method.

If more than one class is deleted from the table in the Class tab of a classification method, the usage assignments for the standards listed in Standards tab will be incorrect.

Calibration results table contains incorrect entries when the number of standards is large and the number of classes is large.

If you create a classification method where the product of the number of standards times the number of classes exceeds 65,536, the last few entries of the calibration results table may contain errors.

TQ Analyst produces an error when the number of classes defined in a classification method is higher than 15.

If you add a class to a classification method that already has fifteen classes, then the method becomes invalid and TQ Analyst is unable to access the method.

PCR method produces memory allocation error when you import standards before defining components.

If you collect or import standards (Standards tab) and then save and close the method without defining the components (Components tab), TQ Analyst may produce a memory allocation error. The error will occur after you reopen the method, select the Standards tab and then select the Components tab.

Known Issues

None

TQ Analyst 6.2

New Features

None

Resolved Issues

Non-zero intercept value was not retained

If you set the Intercept value on the Components tab to Nonzero before defining the method standards and regions, TQ Analyst did not retain the Intercept setting.

Known Issues

The Standards table may have errors in the usage column when more than one class is deleted from a method.

If more than one class is deleted from the table in the Class tab of a classification method, the usage assignments for the standards listed in Standards tab will be incorrect.

Delete only one class each time you enter into the Class tab. Multiple classes can be deleted by exiting the Class tab, reentering the tab and subsequently deleting only one class. You can repeatedly reenter the tab and delete another class without causing a problem with the usage settings.

Calibration results table contains incorrect entries when the number of standards is large *and* the number of classes is large.

If you create a classification method where the product of the number of standards times the number of classes

exceeds 65,536, the last few entries of the calibration results table may contain errors.

The problem affects only the last few entries in the calibration table; the method calibration model remains accurate. To work around the problem, either use fewer standards or decrease the number of classes.

TQ Analyst produces an error when the number of classes defined in a classification method is higher than 15.

If you add a class to a classification method that already has fifteen classes, then the method becomes invalid and TQ Analyst is unable to access the method.

If you create a classification method with fifteen or sixteen classes, the method will work properly. The problem occurs if you open a method that has fifteen classes and then add another class. If you need to add a class to a method that has fifteen classes, create a method with sixteen classes instead of adding a class to the saved method.

PCR method produces memory allocation error when you import standards before defining components

When creating a principal component regression (PCR) method, if you collect or import standards (Standards tab) and then save and close the method before defining the components (Components tab), TQ Analyst produces a memory allocation error when you reopen the method, select the Standards tab and then select the Components tab. If you choose Cancel in the error dialog box, the software exits. If you choose OK instead of Cancel, the error dialog box remains on the screen.

When creating a PCR method, make sure you define the method components before collecting or importing the standards.

Region selection tools sometimes operate improperly when Explain Help window is displayed

The tools for setting region endpoints in the Region Selection task window don’t always operate correctly when the Explain Help window is displayed. You can move the region endpoints by clicking with the mouse, but when you release the mouse button, the endpoints don’t stay put. If you try to move the cursor to another area of the task window, the cursor won’t move past the edge of the graphical plot.

If the cursor doesn’t operate correctly in the graphical portion of the Region Selection task window, choose Ctrl+Alt+Delete, select the Explain Help window in the list of programs to close and then choose End Task.

Winhlp32.exe error message

After you install and then start TQ Analyst software, it may display an error message like the following: "Winhlp32.exe has generated errors and will be closed by Windows. You will need to restart."

If the error message described above appears after you start TQ Analyst, choose OK to close the message window and then ignore it.

TQ Analyst sometimes fails to register a change in the software

If you change a parameter setting in TQ Analyst, the software sometimes doesn’t register the change. For

example, if you select another tab and then reselect the tab that was changed, the parameter will be back to the original setting.

If the software doesn't recognize a new parameter setting, reset the parameter and then make another action on that tab, such as clicking an entry box, to register the change. If you change to another tab and then reselect the tab that was changed, you will see that the parameter is set correctly.

ACLS method with mean centering gives incorrect results when predicted with RESULT 1.1 and 1.0

If you use TQ Analyst 6.2 to create an ACLS method that has the Mean Centering check box selected on the Other tab and then use the method to predict concentration values in an unknown sample, the method works correctly. However, if you link the method to a workflow created in RESULT 1.1 or 1.0 and then use the workflow to predict the concentration values of the same sample, the prediction results will not match the results produced by TQ Analyst.

If you plan to link an ACLS method that uses mean centering to a RESULT workflow, you will need to use RESULT 1.2 or greater. Workflows run in RESULT 1.1 or earlier ignore mean centering in ACLS methods.

Multiple Quantify does not display the correct data in Excel if Quantify.xls is open

When you choose the Multiple Quantify command in the Diagnostics menu, TQ Analyst calculates the results and displays them in an Excel spreadsheet file named Quantify.xls. If Quantify.xls contains data generated the last time you ran Multiple Quantify, the software overwrites those results. However, if you open Quantify.xls in Excel and then run Multiple Quantify from TQ Analyst, Excel does not display the new data. It either moves the Quantify.xls window to the foreground or displays a message indicating the file already exists and asking if you want to overwrite the previous data. If you choose OK in the message dialog box, Excel still does not display the new data.

Close the file Quantify.xls before running the Multiple Quantify command in TQ Analyst.

External Validation does not display the correct data in Excel if Valid.xls is open

When you choose the External Validation command in the Diagnostics menu, TQ Analyst calculates the validation results and displays them in an Excel spreadsheet file named Valid.xls. If Valid.xls contains data generated the last time you ran External Validation, the software overwrites those results. However, if you open Valid.xls in Excel and then run External Validation from TQ Analyst, Excel does not display the new data. It either moves the Valid.xls window to the foreground or displays a message indicating the file already exists and asking if you want to overwrite the previous data. If you choose OK in the message dialog box, Excel still does not display the new data.

Close the file Valid.xls before running the External Validation command in TQ Analyst.

Pasting rows cut from the standards table does not work correctly

If you open a method in TQ Analyst, select one or more rows in the Standards table, perform a Cut command and then paste the data elsewhere in the same Standards table or into the Standards table for another TQ Analyst method, the values in the pasted rows may not match the values in the rows that you cut

Do not cut and paste data in the Standards table. If you want to create a method with a set of

standards that are similar to the standards in an existing method, save the existing method with a new file name and then edit the entries in the Standards table.

Qualitative analysis type suggestion is not automatically set in method

If you run the Analysis Type wizard (by choosing the Suggest Analysis Type Button on the Description tab in the TQ Analyst main window) and then follow the path for qualitative methods, the wizard runs successfully but does not set the Analysis Type to the recommended option when it is finished, as it does for quantitative methods.

After running the Analysis Type wizard for qualitative methods, manually set the Analysis Type to the option recommended by the wizard.

Explain Help text is not fully displayed

Occasionally, the text in the Explain help window is cut off at the bottom and the window does not have a scroll bar.

If the text is cut off and the window does not include a scroll bar, resize the window so that all of the text is visible or the scroll bar appears.

Description field is truncated

The description field on the General tab allows the user to enter more than 250 characters, but only 250 characters are actually retained with the method.

Restrict the text in the Description field to 250 characters.

User specified correction coefficients are recalculated when you display the Corrections window

If you replace one or more of the correction curve coefficients displayed in the Corrections window with a new value and then save and close the window, the method will use the coefficients you entered. If you redisplay the Corrections window (by choosing Edit Corrections on the Corrections tab), TQ Analyst recalculates all of the correction curve coefficients and may replace the previous values.

Reenter the desired correction curve coefficients by hand whenever you display the Corrections window.

FAQ

When I choose Print in TQ Analyst, why doesn’t it print?

If you don’t have a default printer selected in your Windows operating system software, TQ Analyst will not print or display an error message that it is unable to print. Selecting a default printer corrects the problem. For information on how to select a default printer, see the documentation that came with your Windows software.

When I open an example method in TQ Analyst, why are all the parameters unavailable (grayed) in the software?

Your TQ Analyst software includes example methods and corresponding on-line tutorials to demonstrate creating a method for each analysis type. The example methods are provided as "read-only" files. If you want

to run an example method or simply change certain parameter settings to try them out, first save the file with a new file name.

Why does the tab key skip columns in a table?

The tab key navigates proportionally through the columns in a table. If the columns widths vary, the tab key moves the same distance causing it to skip some shorter columns.

Use the arrow keys to move to the next or previous column in a table.

Why are the points in the cross validation plot offset from the diagonal line?

If a TQ Analyst quantitative method includes corrections (see the Corrections tab), the calibration window always reports corrected values for the method standards while the Cross Validation diagnostic (used to identify outliers) reports uncorrected values. This may cause the points in the cross validation plot to be offset from the diagonal line. The Cross Validation diagnostic uses uncorrected values to ensure that outliers can be identified even when the user has selected an over fit correction model.

Why can’t I view derivative data when using a derivative region type?

You cannot view derivative spectra when Region Type (see the Regions tab) is set to 1st Derivative In Range or 2nd Derivative In Range.

These Region Type options are provided to remain compatible with earlier versions of TQ Analyst software. If you want to work with derivative spectra and your method does not need to be compatible with an earlier method, we recommend using the processing features on the Spectra tab to generate the derivative spectra. The Spectra tab is a new feature in 6.0.

How do I view derivatives or smoothed data in spectral diagnostics?

In default mode, spectral diagnostics such as Pure Component Spectra show the original spectra, even if those spectra have been processed, for example by creating derivatives or smoothing.

To view the processed spectra in diagnostic, Region Selection, and other windows in TQ Analyst software, select the Show Processed Spectra In View Standards check box on the Standards tab.

Why does the Save Method dialog box appear when I close a method, even when the method has not changed?

In some situations, TQ Analyst may prompt you to save your method when you have not made any changes. To ensure consistency, TQ Analyst is designed to reset key parameters when you display certain tabs in the TQ Analyst main window. When this occurs, TQ Analyst considers the method modified, even when those parameters are reset to the previously selected option or value.

If the Save Method dialog box appears when closing a method with no changes, you do not need to resave the method (choose Cancel in the Save Method dialog box to leave the method unchanged).

TQ Analyst 6.1a

New Features

None

Resolved Issues

Performing merge standards on a method that was read-only left the method in an inconsistent state

If you used the Merge Standards command on a method file that had read-only access, TQ Analyst created the new merged standard but couldn’t properly save it with the method. As a result, the program set the usage for the merged standard to "Unassigned" and left the method in an inconsistent state. If you performed further operations on the method, you may have encountered a bad memory pointer error.

Canceling a cross validation operation sometimes required two steps and left the method uncalibrated

If you opened a method and ran the Cross Validation command and then chose the Cancel button in the Cross Validation dialog box, the cross validation operation started anyway. If you chose Cancel again in the Cross Validation status dialog box, cross validation ended but left the method uncalibrated.

Assess feasibility wizard caused runtime error number 91

After running the Assess Feasibility wizard, if you chose the Next button two times in succession, the wizard generated runtime error number 91 and stopped running.

Linear Removed baseline option for SNV pathlength correction applied quadratic removed baseline correction instead

When the Standard Normal Variate (SNV) pathlength correction option was selected for a Stepwise Multiple Linear Regression (SMLR) method, TQ Analyst performed quadratic baseline removal even if the linear baseline removal option was selected.

Spectra collected from a tablet analyzer were truncated at 8.0 absorbance units

The detectors on the tablet analyzer could measure absorbance values above 6.0 absorbance units; however, the software truncated all absorbance values to 6.0 absorbance units. On detectors other than the tablet analyzer, this truncation did not change the region choice, as measurements above 6.0 absorbance units are non-linear and not suitable for qualitative or quantitative work.

Avoid regions with data at or above 6.0 absorbance units measured by a tablet analyzer.

Conversion from Discriminant Analysis to QC Compare Search analysis type prevented proper calibration

If you created a discriminant analysis method, added standards to it, and then converted it to a QC Compare Search method, you were not able to properly calibrate the new method and TQ Analyst reported all materials as belonging to the same class.

Known Issues

Region selection tools sometimes operate improperly when Explain Help window is displayed

The tools for setting region endpoints in the Region Selection task window don't always operate correctly when the Explain Help window is displayed. You can move the region endpoints by clicking with the mouse, but when you release the mouse button, the endpoints don't stay put. If you try to move the cursor to another area of the task window, the cursor won't move past the edge of the graphical plot.

If the cursor doesn't operate correctly in the graphical portion of the Region Selection task window, choose Ctrl+Alt+Delete, select the Explain Help window in the list of programs to close and then choose End Task.

TQ Analyst sometimes fails to register a change in the software

If you change a parameter setting in TQ Analyst, the software sometimes doesn't register the change. For example, if you select another tab and then reselect the tab that was changed, the parameter will be back to the original setting.

If the software doesn't recognize a new parameter setting, reset the parameter and then make another action on that tab, such as clicking an entry box, to register the change. If you change to another tab and then reselect the tab that was changed, you will see that the parameter is set correctly.

Multiple Quantify does not display the correct data in Excel if Quantify.xls is open

When you choose the Multiple Quantify command in the Diagnostics menu, TQ Analyst calculates the results and displays them in an Excel spreadsheet file named Quantify.xls. If Quantify.xls contains data generated the last time you ran Multiple Quantify, the software overwrites those results. However, if you open Quantify.xls in Excel and then run Multiple Quantify from TQ Analyst, Excel does not display the new data. It either moves the Quantify.xls window to the foreground or displays a message indicating the file already exists and asking if you want to overwrite the previous data. If you choose OK in the message dialog box, Excel still does not display the new data.

Close the file Quantify.xls before running the Multiple Quantify command in TQ Analyst.

External Validation does not display the correct data in Excel if Valid.xls is open

When you choose the External Validation command in the Diagnostics menu, TQ Analyst calculates the validation results and displays them in an Excel spreadsheet file named Valid.xls. If Valid.xls contains data generated the last time you ran External Validation, the software overwrites those results. However, if you open Valid.xls in Excel and then run External Validation from TQ Analyst, Excel does not display the new data. It either moves the Valid.xls window to the foreground or displays a message indicating the file already exists and asking if you want to overwrite the previous data. If you choose OK in the message dialog box, Excel still does not display the new data.

Close the file Valid.xls before running the External Validation command in TQ Analyst.

Pasting rows cut from the standards table does not work correctly

If you open a method in TQ Analyst, select one or more rows in the Standards table, perform a Cut command and then paste the data elsewhere in the same Standards table or into the Standards table for another TQ

Analyst method, the values in the pasted rows may not match the values in the rows that you cut

Do not cut and paste data in the Standards table. If you want to create a method with a set of standards that are similar to the standards in an existing method, save the existing method with a new file name and then edit the entries in the Standards table.

Qualitative analysis type suggestion is not automatically set in method

If you run the Analysis Type wizard (by choosing the Suggest Analysis Type Button on the Description tab in the TQ Analyst main window) and then follow the path for qualitative methods, the wizard runs successfully but does not set the Analysis Type to the recommended option when it is finished, as it does for quantitative methods.

After running the Analysis Type wizard for qualitative methods, manually set the Analysis Type to the option recommended by the wizard.

Explain Help text is not fully displayed

Occasionally, the text in the Explain help window is cut off at the bottom and the window does not have a scroll bar.

If the text is cut off and the window does not include a scroll bar, resize the window so that all of the text is visible or the scroll bar appears.

Non-zero intercept value is not retained

If you set the Intercept value on the Components tab to Nonzero before defining the method standards and regions, TQ Analyst does not retain the Intercept setting.

Set all other values in your method before returning to the Components tab and setting the Intercept to Nonzero.

Description field is truncated

The description field on the General tab allows the user to enter more than 250 characters, but only 250 characters are actually retained with the method.

Restrict the text in the Description field to 250 characters.

User specified correction coefficients are recalculated when you display the Corrections window

If you replace one or more of the correction curve coefficients displayed in the Corrections window with a new value and then save and close the window, the method will use the coefficients you entered. If you redisplay the Corrections window (by choosing Edit Corrections on the Corrections tab), TQ Analyst recalculates all of the correction curve coefficients and may replace the previous values.

Reenter the desired correction curve coefficients by hand whenever you display the Corrections window.

FAQ

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If you don't have a default printer selected in your Windows operating system software, TQ Analyst will not print or display an error message that it is unable to print. Selecting a default printer corrects the problem. For information on how to select a default printer, see the documentation that came with your Windows software.

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Use the arrow keys to move to the next or previous column in a table.

Why are the points in the cross validation plot offset from the diagonal line?

If a TQ Analyst quantitative method includes corrections (see the Corrections tab), the calibration window always reports corrected values for the method standards while the Cross Validation diagnostic (used to identify outliers) reports uncorrected values. This may cause the points in the cross validation plot to be offset from the diagonal line. The Cross Validation diagnostic uses uncorrected values to ensure that outliers can be identified even when the user has selected an over fit correction model.

Why can't I view derivative data when using a derivative region type?

You cannot view derivative spectra when Region Type (see the Regions tab) is set to 1st Derivative In Range or 2nd Derivative In Range.

These Region Type options are provided to remain compatible with earlier versions of TQ Analyst software. If you want to work with derivative spectra and your method does not need to be compatible with an earlier method, we recommend using the processing features on the Spectra tab to generate the derivative spectra. The Spectra tab is a new feature in 6.0.

How do I view derivatives or smoothed data in spectral diagnostics?

In default mode, spectral diagnostics such as Pure Component Spectra show the original spectra, even if those spectra have been processed, for example by creating derivatives or smoothing.

To view the processed spectra in diagnostic, Region Selection, and other windows in TQ Analyst software, select the Show Processed Spectra In View Standards check box on the Standards tab.

Why does the Save Method dialog box appear when I close a method, even when the method has not changed?

In some situations, TQ Analyst may prompt you to save your method when you have not made any changes. To ensure consistency, TQ Analyst is designed to reset key parameters when you display certain tabs in the TQ Analyst main window. When this occurs, TQ Analyst considers the method modified, even when those parameters are reset to the previously selected option or value.

If the Save Method dialog box appears when closing a method with no changes, you do not need to resave the method (choose Cancel in the Save Method dialog box to leave the method unchanged).

TQ Analyst 6.1

New Features
None

Resolved Issues
None

Known Issues

Region selection tools sometimes operate improperly when Explain Help window is displayed
The tools for setting region endpoints in the Region Selection task window don't always operate correctly when the Explain Help window is displayed. You can move the region endpoints by clicking with the mouse, but when you release the mouse button, the endpoints don't stay put. If you try to move the cursor to another area of the task window, the cursor won't move past the edge of the graphical plot.

If the cursor doesn't operate correctly in the graphical portion of the Region Selection task window, choose Ctrl+Alt+Delete, select the Explain Help window in the list of programs to close and then choose End Task.

TQ Analyst sometimes fails to register a change in the software
If you change a parameter setting in TQ Analyst, the software sometimes doesn't register the change. For example, if you select another tab and then reselect the tab that was changed, the parameter will be back to the original setting.

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Close the file Valid.xls before running the External Validation command in TQ Analyst.

Performing merge standards on a method that is read-only leaves method in an inconsistent state

If you use the Merge Standards command on a method file that has read-only access, TQ Analyst creates the new merged standard but cannot properly save it with the method. As a result, the program sets the usage for the merged standard to "Unassigned" and leaves the method in an inconsistent state. If you perform further operations on the method, you may encounter a bad memory pointer error.

Make sure the method has read/write access before using Merge Standards.

Canceling a cross validation operation may require two steps and leaves method uncalibrated

If you open a method and run the Cross Validation command and then choose the Cancel button in the Cross Validation dialog box, the cross validation operation starts anyway. If you choose Cancel again in the Cross Validation status dialog box, cross validation ends but leaves the method uncalibrated.

Cancel the cross validation in both dialog boxes and then recalibrate the method to leave it in the previous state.

Pasting rows cut from the standards table does not work correctly

If you open a method in TQ Analyst, select one or more rows in the Standards table, perform a Cut command and then paste the data elsewhere in the same Standards table or into the Standards table for another TQ Analyst method, the values in the pasted rows may not match the values in the rows that you cut

Do not cut and paste data in the Standards table. If you want to create a method with a set of standards that are similar to the standards in an existing method, save the existing method with a new file name and then edit the entries in the Standards table.

Assess feasibility wizard causes runtime error number 91

After running the Assess Feasibility wizard, if you choose the Next button two times in succession, the wizard generates runtime error number 91 and stops running.

Linear Removed baseline option for SNV pathlength correction applies quadratic removed baseline correction instead

When the Standard Normal Variate (SNV) pathlength correction option is selected for a Stepwise Multiple Linear Regression (SMLR) method, TQ Analyst performs quadratic baseline removal even if the linear baseline removal option is selected.

Select the Quadratic Removed baseline option when using the SNV pathlength correction in an SMLR method, since this is the calculation that is actually performed. The method's prediction results using a Linear Removed baseline correction option will be reasonable; however, the baseline will be corrected with a quadratic and not a linear baseline.

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After running the Analysis Type wizard for qualitative methods, manually set the Analysis Type to the option recommended by the wizard.

Avoid regions with data at or above 6.0 absorbance units measured by a tablet analyzer

The detectors on the tablet analyzer can measure absorbance values above 6.0 absorbance units; however, the software truncates all absorbance values to 6.0 absorbance units. On detectors other than the tablet analyzer, this truncation would not change your region choice, as measurements above 6.0 absorbance units are non-linear and not suitable for qualitative or quantitative work.

Perform your measurement in regions that don't meet or exceed 6.0 absorbance units.

Conversion from Discriminant Analysis to QC Compare Search analysis type may prevent proper calibration

If you create a discriminant analysis method, add standards to it, and then convert it to a QC Compare Search method, you may not be able to properly calibrate the new method and TQ Analyst may report all materials as belonging to the same class.

Review the data displayed in the Calibration Results window whenever you calibrate a qualitative (classification) method to ensure that the software predicts the proper class for each of the method standards. If the software predicts all or most of the method standards incorrectly, it may have encountered this calibration error.

If the error occurs in an existing classification method, recreate the method. If you are creating a new classification method, select the QC Compare Search analysis type and add the first standard to the method. Once the method contains at least one standard, you can switch between the QC Compare Search, Discriminant Analysis, and other classification method types without a problem.

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How to Contact Us

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