# **Product Overview** TQ Analyst Software Chemometric Algorithms

Thermo Scientific TQ Analyst is a chemometric software package that is very flexible and extremely easy to use. Primary chemometric algorithms are divided into Quantitative and Qualitative analysis. Below is a list and brief description of these primary chemometric analysis algorithms.

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# **Quantitative Analysis**

## **Beer's Law**

Simple Beer's Law is a quantitative analysis technique based on Beer's Law. Select the Simple Beer's Law analysis type when each of the components you want to measure produces a unique peak in the spectrum of the sample mixture. The component peaks must contain little or no absorptions from other components in the sample. If the component peaks overlap significantly or do not increase proportionally with concentration, use the CLS analysis type instead of Simple Beer's Law.

## **Classical Least Squares (CLS)**

Classical Least Squares is a quantitative analysis technique based on the least squares algorithm. Select the CLS analysis type when each component you want to measure produces a peak or combination of peaks in the spectrum of the sample mixture, but the component peaks overlap significantly. If the component peaks overlap severely or if molecular interactions between components are affecting the absorbance in the regions you want to measure, use the Partial Least Squares (PLS) analysis type rather than Classical Least Squares.

## **Stepwise Multiple Linear Regression**

The stepwise multiple linear regression (SMLR) technique expresses concentration as a function of the absorbance at multiple frequencies. This is the opposite (inverse) of the classical least squares technique where absorbance is a function of concentration. Select the SMLR analysis type when you are interested in measuring the concentrations of a few components in a multi-component mixture. SMLR works well when there is little or no overlap between component peaks and the components of interest absorb linearly with concentration. Since SMLR expresses concentration as a function of the absorbance at multiple frequencies, it is not necessary to account for every component or interference in the sample mixture.

# Partial Least Squares

Partial Least Squares (PLS) is a statistical approach to quantitative analysis based on the partial least squares algorithm. Select the PLS analysis type when each component you want to measure produces a measurable peak in the spectrum of the sample mixture but the component peaks overlap severely. A PLS method is capable of quantifying sample components when the correlation between concentration and absorbance is very complex. Since PLS is a statistical analysis technique, a large number of standards are needed in order to correlate spectral information with concentration.

## **Principal Component Regression**

Principal Component Regression (PCR) is another statistical quantitative analysis technique based on the principal component regression algorithm. The PCR algorithm frequently requires one or two more factors to describe spectral variation than the PLS algorithms does so it may take longer to calibrate a PCR method. In addition, all of the components in a PCR method must be measured in each region.



# **Classification (Qualitative Analysis)**

#### **Similarity Match**

Similarity match is a spectral classification technique that indicates how closely an unknown material matches a known material. The Similarity Match algorithm is typically used for quality control applications. In these applications, the desired composition of the samples is known and the analyst is interested in verifying the samples or identifying when impurities are present.

### **Distance Match**

The Distance Match classification technique can be used to determine how closely an unknown material matches two or more classes of known materials by calculating a conformity spectrum for each class and measuring its distance from the class average. This technique is typically used to screen incoming materials to determine how closely they match known compounds or to determine "degrees of difference" between known and unknown materials. The Distance Match algorithm works well for differentiating materials that contain different amounts of the same components.

#### **Discriminant Analysis and SIMCA**

The Discriminant Analysis classification technique is a PCA-based algorithm and can be used to determine the class or classes of known materials which are most similar to an unknown material by computing the unknown's distance from each class center in Mahalanobis distance units. The discriminant analysis technique is typically used to screen incoming materials where the analyst is interested in identifying which known material each sample is most like. Soft Independent Modeling of Class Analogy (SIMCA) is also available for use in this technique.

#### **Search Standards**

Search Standards is a spectral classification technique that determines the known materials which are most similar to an unknown material. One standard is used to describe each known material. Select the Search Standards analysis type if you want to compare an unknown material with many known materials.

#### **QC** Compare search

QC Compare Search is a spectral classification technique that determines the single best match from each class and indicates how closely the unknown material matches the spectrum of the chosen standard. The method must specify at least two classes of known materials. Multiple standards may be used to describe each class. Multiple regions of the spectrum may be used for the analysis. The QC Compare Search algorithm can be used to verify the composition of an unknown material that is known to belong to one of several classes. In these applications, the analyst is interested in identifying which known material each sample is most like.

## Measurement

#### **Measurement Only**

Select the Measurement Only analysis type when you need to report measured peak heights or areas, peak locations, peak widths, noise values, the ratio of two measured peaks, or measured values that have been adjusted with a multiplicative factor or offset ratios. No calibration model is created for a spectral measurement method.

Additional Algorithms

In addition to the primary algorithms described above, TQ Analyst<sup>™</sup> software uses an exceptionally large number of features that allow a areat deal of control over data and chemometric analysis. Below is a list of the various algorithms and parameters available with the software package that provides an unprecedented amount of direction over chemometric methods used in spectroscopic analysis.

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85. Noise

70. Loading Value

Match Type

Mahalanobis Distance

Match Value Check

Maxi-Min Strategy

Mean Spectrum

Pathlength Type

Non-linear PLS

Maximum Components Per Search

Maximum Height in Range Region Type

Measurement Region Spectrum Check

Minimum Height in Range Region Type

Multiple Correlation Spectrums

Multiplicative Signal Correction

Multipoint Baseline Correction

Minimum Height in Range Baseline Type

Maximum Height in Range Baseline Type

- Absolute Derivative 1
- Absolute Derivative Search 2. 3
- Absolute Difference Absolute Difference Search 4

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- Absolute Maximum in Range
- Acceptance Limits Check
- 7. Analysis Limits Check
- 8. Analysis Type parameter
- 9. Analysis of Variance
- 10. Augmented Classical Least Squares
- Average Distance Ratio Performance Check 11
- 12. Average Height in Range
- 13. Average in Range Baseline
- 14. **Baseline Corrected Measurement**
- 15. Baseline Location
- 16. Baseline Offset
- 17. Baseline Type (Pathlength)
- Baseline Type-lower 18.
- 19 Baseline Type-upper
- 20. Center of Gravity Peak Location
- 21 Chauvenet test
- 22. Computed Area Region Type
- 23 Constant Pathlength
- 24. Correction Coefficient
- 25. **Correlation Coefficient**
- 26. **Correlation Option**
- Correlation Search 27
- 28. Cross Correction
- 29 Cross Validation Component PI
- 30. Cross Validation PI
- 31. Cumulative Residual Spectrum
- 32. **Dilution Factor**
- 33. **Distance Value Check** 34. Dixon Test
- Edit Regions (SMLR) 35
- 36. Enhance Correlation Metric
- 37. Euclidean Distance from Zero
- 38. Extraction Factor
- 39. F ratio
- 40. Factorial Design
- 41 Find Residual Differences
- 42. Find Similarities 43. First Derivative
- 44. First Derivative in Range 45. Fit Value Algorithm
- Fixed Location Baseline 46.
- 47. Fixed Location Height
- 48. Force Through Zero Parameter
- 49. Fractional Factorial Design Model
- 50. Full Factorial Design Model
- 51. Full Spectrum Fit Value
- 52. Full Spectrum Check
- 53. Full Width Half Height
- 54. Galactic-Type Correlation 55.
- Internal Reference Pathlength Type 56. Interpolated Height at Exact Location
- Known Pathlength Type 57.
- 58. Least Squares
- 59 Leverage Value
- 60. Linear Correction
- 61. Linear Removed Baseline Type
- 62 Linear Filters
- 63. Location at Percent of Peak Max
- 64. Location at Peak Max Region Type
- 65. Location of Maximum Height in Range Location of Minimum Height in Range
- 66. Location of Match Height (Low) 67
- 68 Location of Match Height (High)
- 69. Location Parameters

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- 87 Norris Derivative Smoothing 88. One Point Baseline Type 89 Peak Height Peak Height Interpolated Region 90. 91. Peak Location Interpolated Region 92. Peak Width at Percent of Maximum 93 Peak Width Low Location referenced 94 Peak Width High Location Referenced 95 Peak Width at Half Max 96 Peak Ratio Pathlength Type 97. Peak-to-Peak Noise 98. Percent Difference 99. Percent or Height Parameter 100. Performance Index 101. Piecewise Linear Correction 102. Predict Pathlength Type 103. Pure Component Spectrum 104. Quadratic Removed Baseline 105. Random Design 106. Region Type 107. Residual Concentration Error 108. Residual Spectrum 109. Restrict Y-Axis Range for Samples 110. Root Mean Square Error 111. Root Mean Square Noise 112. Savitsky-Golay Filter 113. Score Value 114. Search Type 115. Second Derivative 116. Sensitive Fit Value 117. Simple Fit Value 118. Signal-to-Noise Ratio
- 119. Soft Independent Modeling of Class Analogy
- 120. Spectral Range Parameter
- 121. Spline Correction
- 122. Squared Derivative
- 123. Squared Difference
- 124. Standard Deviation
- 125. Standard Error Check
- 126. Standard Normal Variate Pathlength

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- 127. Subtraction Factor
- 128. Threshold Distance Value
- 129. Threshold F ratio 130. Threshold Fit value
- 131. Threshold match value

134. Uncertainty Limit 135. Uncertainty Value Check

136. Variance Spectrum

- 132. Trend Line Slope Region Type
- 133. Two Point Baseline Type