

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.

The screenshot shows a Microsoft Excel spreadsheet with the following content:

1

2 **Quantitative analysis by Simple Beer's Law**

3 In Beer's law analysis, the absorbance of a component at a particular frequency is assumed to be caused by a single component.

4 The challenge is to find a frequency that is free of outside interferences (such as other components)

5 and that best (most linearly) describes the amount of component present.

6 For this problem the measurement is made at 5957.80 cm⁻¹ corrected for a baseline drawn horizontally

7 The intensity at 5957.80 cm⁻¹ is determined from a three point, Lagrangian interpolation.

8 The baseline is the intensity at the data point nearest to 6382.94 cm⁻¹

9 The calibration step uses a set of standards of known concentration to solve the equation: $A = k \cdot C$. The unknown in the equation

10 For this problem there are 20 standards with known concentrations.

11 During prediction you know A (from the spectrum) and k (from the calibration step). This allows you to solve for C, the unknown co

12

13 The expected answer is 2.9267

14 The answer is in spreadsheet entry C83 2.926663087

15

16

	Standard 1	Standard 2	Standard 3	Standard 4	Standard 5	Standard 6	Standard 7
17 Concentration	1.0	2.0	3.0	4.0	5.0	1.0	1.0
18 Frequency	5943.534535	0.493664	0.988529	1.48044	2.01009	2.48705	0.486617
19	5947.391469	0.496217	0.993706	1.48762	2.01964	2.50341	0.489192
20	5951.249402	0.49516	0.991471	1.48443	2.01267	2.49507	0.489354
21	5955.105335	0.493902	0.9875	1.47536	2.00611	2.48889	0.488314
22	5958.967269	0.489321	0.981393	1.4695	1.99328	2.45792	0.482326

23 Point just before the target

24 Point closest to the target

Ready

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™ software uses an exceptionally large number of features that allow a great 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.

1. Absolute Derivative
2. Absolute Derivative Search
3. Absolute Difference
4. Absolute Difference Search
5. Absolute Maximum in Range
6. Acceptance Limits Check
7. Analysis Limits Check
8. Analysis Type parameter
9. Analysis of Variance
10. Augmented Classical Least Squares
11. Average Distance Ratio Performance Check
12. Average Height in Range
13. Average in Range Baseline
14. Baseline Corrected Measurement
15. Baseline Location
16. Baseline Offset
17. Baseline Type (Pathlength)
18. Baseline Type-lower
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
27. Correlation Search
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
35. Edit Regions (SMLR)
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
46. Fixed Location Baseline
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
57. Known Pathlength Type
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
66. Location of Minimum Height in Range
67. Location of Match Height (Low)
68. Location of Match Height (High)
69. Location Parameters
70. Loading Value
71. Mahalanobis Distance
72. Match Type
73. Match Value Check
74. Maxi-Min Strategy
75. Maximum Components Per Search
76. Maximum Height in Range Region Type
77. Maximum Height in Range Baseline Type
78. Mean Spectrum
79. Measurement Region Spectrum Check
80. Minimum Height in Range Region Type
81. Minimum Height in Range Baseline Type
82. Multiple Correlation Spectrums
83. Multiplicative Signal Correction Pathlength Type
84. Multipoint Baseline Correction
85. Noise
86. Non-linear PLS
87. Norris Derivative Smoothing
88. One Point Baseline Type
89. Peak Height
90. Peak Height Interpolated Region
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
127. Subtraction Factor
128. Threshold Distance Value
129. Threshold F ratio
130. Threshold Fit value
131. Threshold match value
132. Trend Line Slope Region Type
133. Two Point Baseline Type
134. Uncertainty Limit
135. Uncertainty Value Check
136. Variance Spectrum

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