

## Thermo Scientific ValPro for Antaris: TQ Analyst Algorithms

Validation tools for your software and chemometric methods

Thermo Scientific FT-NIR software is verified and validated internally as part of our formalized Product Development Process. This includes verification of:

- RESULT analysis software
- ValPro qualification package
- TQ Analyst software for quantitative analysis
- All algorithms used in the software packages

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

In Beer's law analysis, the absorbance of a component at a particular frequency is assumed to be caused by a single component. The challenge is to find a frequency that is free of outside interferences (such as other components) and that best (most linearly) describes the amount of component present.

For this problem the measurement is made at 5957.80 cm<sup>-1</sup> corrected for a baseline drawn horizontally. The intensity at 5957.80 cm<sup>-1</sup> is determined from a three point, Lagrangian interpolation.

The baseline is the intensity at the data point nearest to 5782.94 cm<sup>-1</sup>.

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

For this problem there are 20 standards with known concentrations.

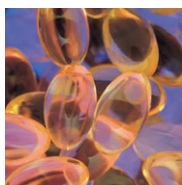
During prediction you know  $A$  (from the spectrum) and  $k$  (from the calibration step). This allows you to solve for  $C$ , the unknown concentration.

The expected answer is 2.9267

The answer is in spreadsheet entry C83: 2.92663067

	Standard 1	Standard 2	Standard 3	Standard 4	Standard 5	Standard 6	Standard 7
Concentration	1.0	2.0	3.0	4.0	5.0	1.0	1.0
Frequency							
5943.534535	0.493664	0.988529	1.48044	2.01009	2.48705	0.486617	
5947.391469	0.496217	0.993708	1.48762	2.01964	2.50341	0.489192	
5951.248402	0.49516	0.991471	1.48443	2.01267	2.49507	0.488054	
5955.115135	0.495802	0.98795	1.47836	2.00801	2.48819	0.489014	
Point element to the target: 5956.962369	0.489921	0.981393	1.46946	1.99326	2.46792	0.482626	

Example spreadsheet of a TQ Analyst™ Algorithms



Our level of extensive testing, as documented in the Thermo Scientific ValPro System Qualification manual, is generally sufficient to satisfy your industry's regulatory requirements for the validation of commercial off-the-shelf (COTS) software. However, in some cases to satisfy more stringent internal requirements, it may be necessary to show regulatory authorities that the algorithms you are using in the analysis of spectroscopic data are producing the answers you expect. We have developed a tool that will allow you to verify mathematical integrity of algorithms utilized in Thermo Scientific TQ Analyst software packages. This powerful verification tool provides:

- Automated algorithm verification
- Confidence in the integrity of your analytical results
- Reduced cost of compliance
- Simplified software algorithm validation
- Reduced time required to validate chemometric models

The following steps are performed in a Principal Component Regression (PCR) calibration for dimensions  $h = 1, 2, \dots, a$ :

1. Initialize a matrix  $\mathbf{U}$  that has  $r$  rows and has  $h = 0$  columns.
2. Increase  $h$  by 1 and select the column of  $\mathbf{X}$  (actually  $\mathbf{X}_h$  because it depends on the value of  $h$ ) with the greatest sum of squares. This is a first estimate for the principal component scores (or latent variables). Call this vector  $\mathbf{u}_h$ . This vector is of size  $r \times 1$ .
3. Compute the squared norm of  $\mathbf{u}_h$ .  
$$\mathbf{u}_h^2 = \mathbf{u}_h^T \mathbf{u}_h$$
4. Calculate the row vector  $\mathbf{b}_h$  as  
$$\mathbf{b}_h^T = \mathbf{u}_h^T \mathbf{X} / \mathbf{u}_h^2$$
  $\mathbf{b}_h$  is of size  $p \times 1$ .

Example documentation of TQ Analyst's PCR Algorithm

The TQ Analyst Algorithms package offers written explanations, including formulas for the algorithms, along with a series of Microsoft® Excel spreadsheets. These spreadsheets can be used as templates to externally validate the algorithms and methods you develop. Over 40 algorithms are described in the documentation and executed in the Excel spreadsheets, including:

- Quantitative algorithms such as classic least squares (CLS) and partial least squares (PLS)
- Qualitative algorithms such as Similarity Match and Distance Match
- Measurement Only methods for measuring peak height and location
- Baseline corrections
- Pretreatments such as derivatives

Thermo Scientific Antaris FT-NIR instrument users in regulated industries who are required to prove validation of processes to auditors will find this tool invaluable.

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