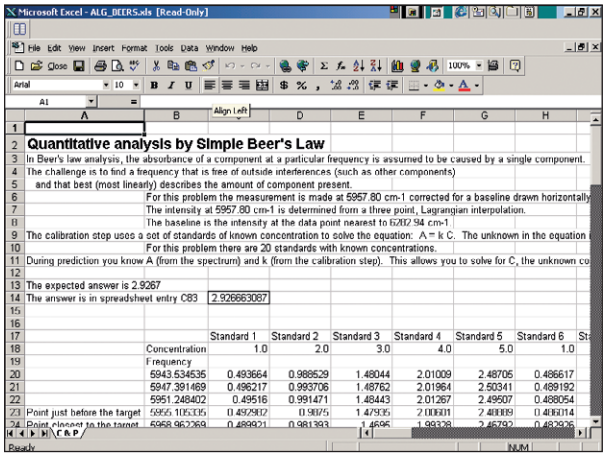
Product Specifications

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

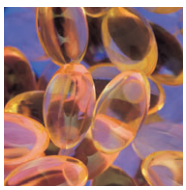
- **RESULT analysis software**
- **ValPro qualification package**
- **TQ Analyst software for quantitative analysis**
- **All algorithms used in the software packages**

Thermo Scientific ValPro for Antaris: TQ Analyst Algorithms

Validation tools for your software and chemometric methods



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 $h = 1, 2, \ldots, a$:

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 $\mathbf{u_h}$ $\mathbf{u_h}$. This vector is of size r x 1.
3. Compute the squared norm of u_h. $u_h^2 = \mathbf{u_h}^1 \mathbf{u_h}$
4. Calculate the row vector b_h as $\mathbf{b_h}^1 = \mathbf{u_h}^1 X / \mathbf{u_h}^2$ $\mathbf{b_h}$ is of size p x 1.

Example documentation of TQ Analyst's PCR Algorithm

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Product Specifications

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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Thermo Electron Scientific Instruments LLC, Madison, WI USA is ISO Certified.

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