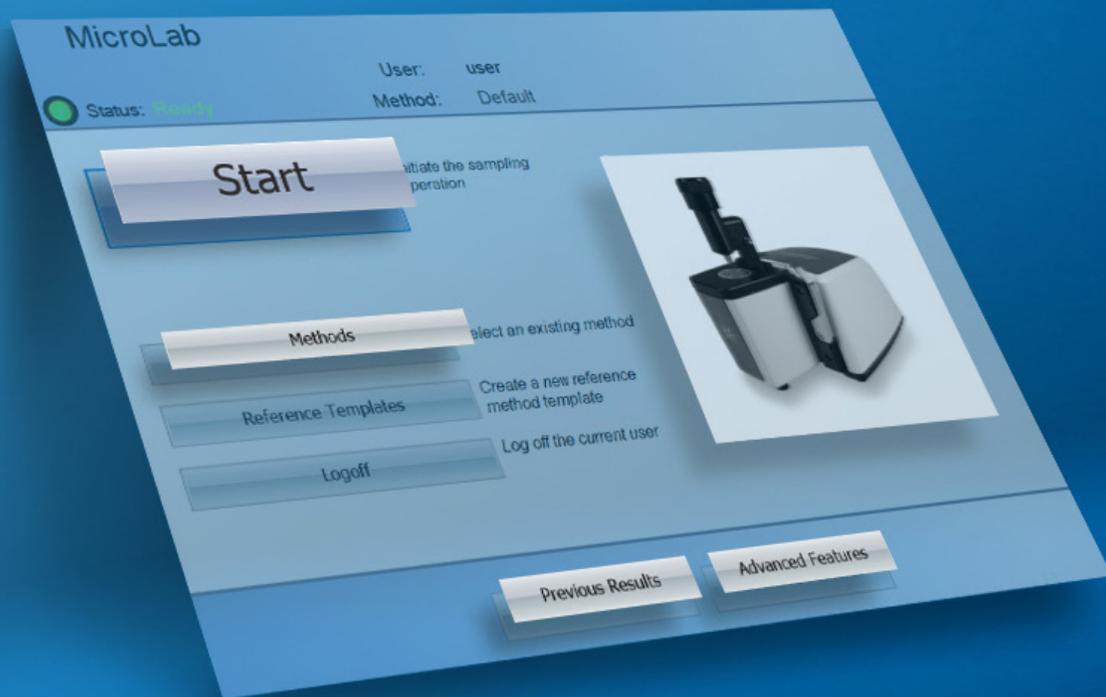


# FTIR Analysis Made Easy

Agilent MicroLab Software



## MicroLab software

Fourier transform infrared spectroscopy (FTIR) is a quick, easy, and reliable technique for material identification and quantification of components in a sample.



Agilent offers a range of FTIR instruments, from flexible, handheld FTIR spectrometers and robust, portable FTIR analyzers for field applications, to reliable benchtop FTIR instruments for routine testing and cutting-edge research. In part, what makes Agilent FTIR spectrometer unique is the software package or interface that accompanies it. Agilent MicroLab software allows users of all levels to use it for routine applications from unknown material identification and characterization to detailed quantitative analysis.



Cary 630 FTIR



4500 Portable FTIR



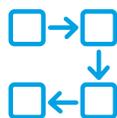
5500 Compact FTIR



4300 Handheld FTIR

Mobile FTIR

## MicroLab software features



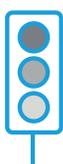
Step-by-step guidance using instructive pictures and an intuitive software design allows easy navigation through the entire workflow, for less training and fewer user mistakes.



MicroLab automatically identifies the connected instrument and recognizes the attached sampling module.



The software directly applies the correct parameters and displays the relevant pictures. Permitted modules can be defined for each method.



Eliminate doubts due to data interpretation from routine workflows: after data collection, the software directly provides color-coded, actionable results, making interpretation simple.



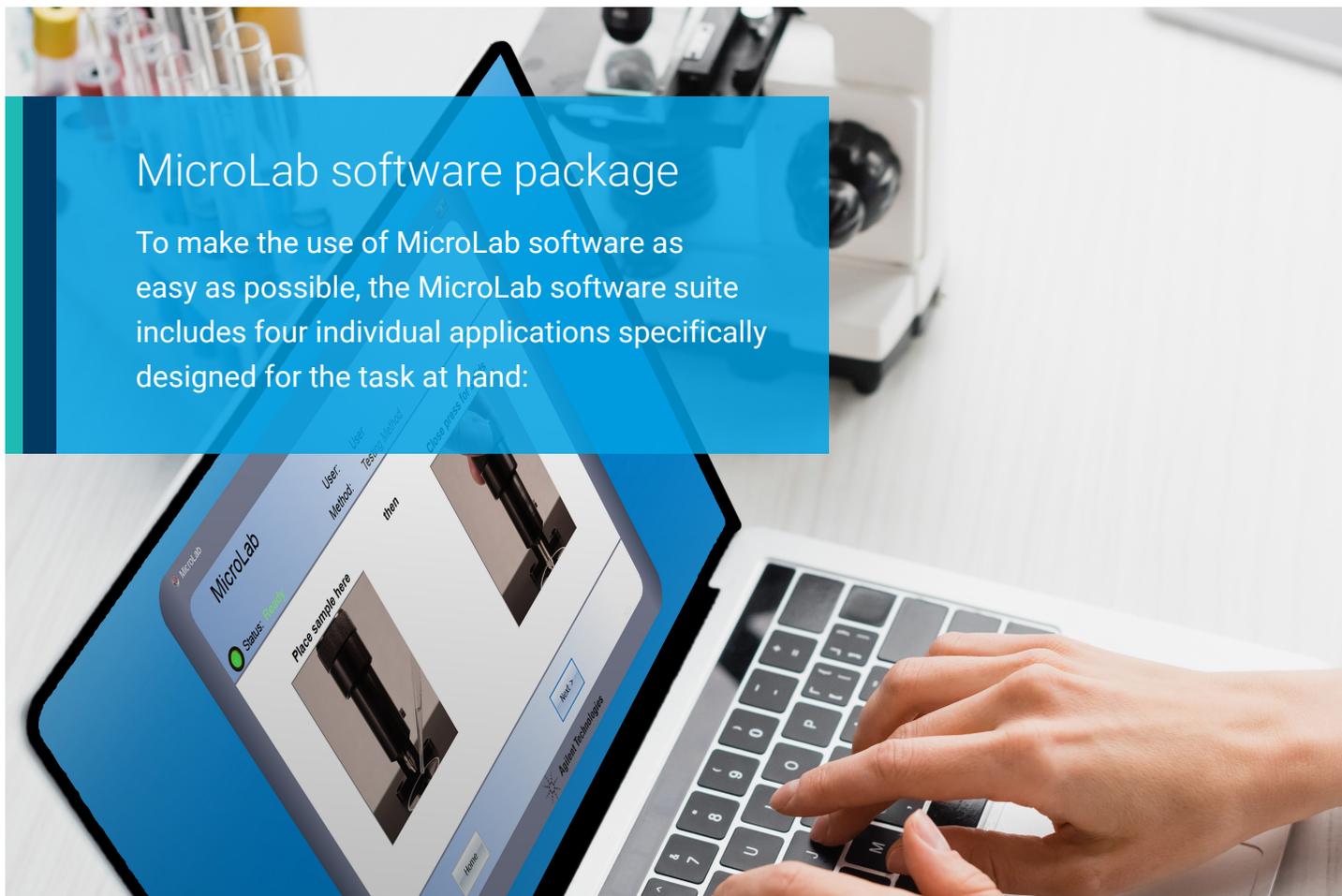
Expand the fast and simple software experience to model development for quantitative applications: MicroLab Quant software assists experts and nonexperts through each step in building a quantitative model, and provides instant feedback when optimizing the model.



Report all relevant results: MicroLab incorporates predefined and customizable report templates. Results can be automatically reported, and a consistent format allows swift review of relevant details.

## MicroLab software package

To make the use of MicroLab software as easy as possible, the MicroLab software suite includes four individual applications specifically designed for the task at hand:



### MicroLab PC

is a method-driven software for collecting and analyzing data using predefined methods.

### MicroLab Lite

software can be used for offline review and analysis of FTIR data.

### MicroLab Quant

used for simple, easy development and verification of quantification models.

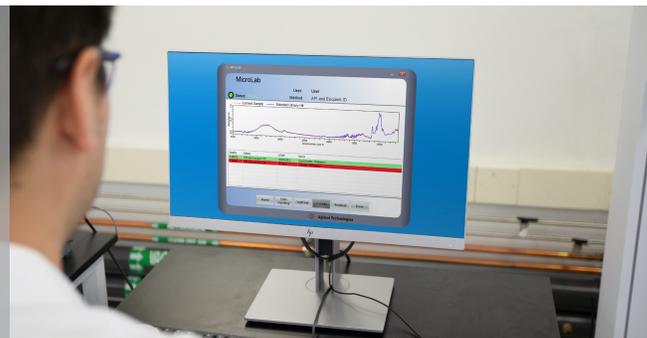
### MicroLab OQ

an automated operational qualification (OQ) software that can be used to routinely verify instrument performance.

The optional **Agilent MicroLab Expert** software is ideal when more sophisticated data processing, visualization, and analysis tools are required.

The **Agilent MicroLab Pharma** software is an additional software solution that allows users to manage user privileges and administer secure storage of electronic records. It also facilitates compliance as defined by U.S. FDA 21 CFR Part 11, EU Annex 11, and similar national electronic record regulations.

# Finding answers with MicroLab PC and MicroLab Lite

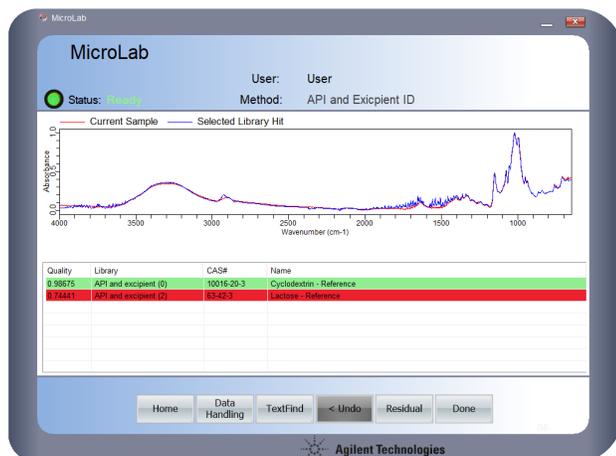


## Software method types

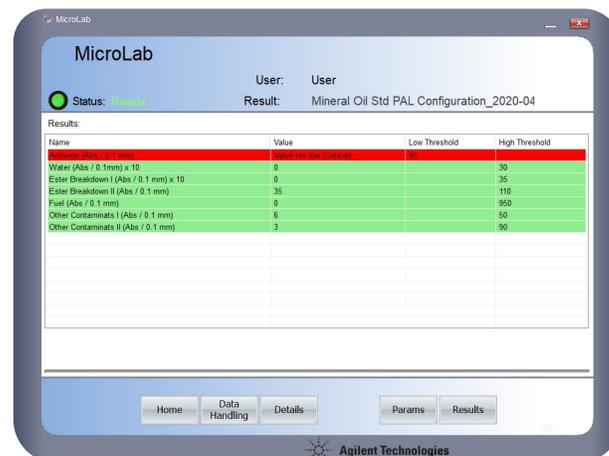
The MicroLab software follows a method-based approach. After the method is set up, the system becomes a turnkey solution.

Three different method types cover the most important analytical questions:

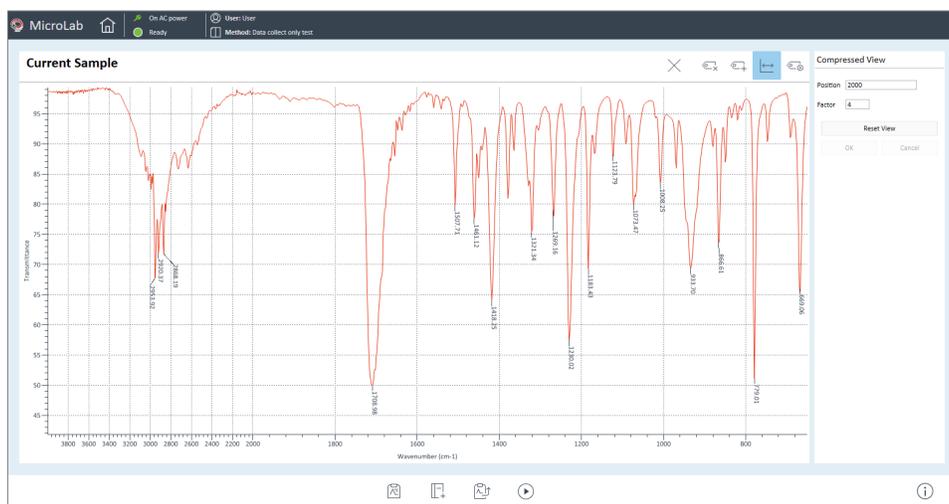
### Identification



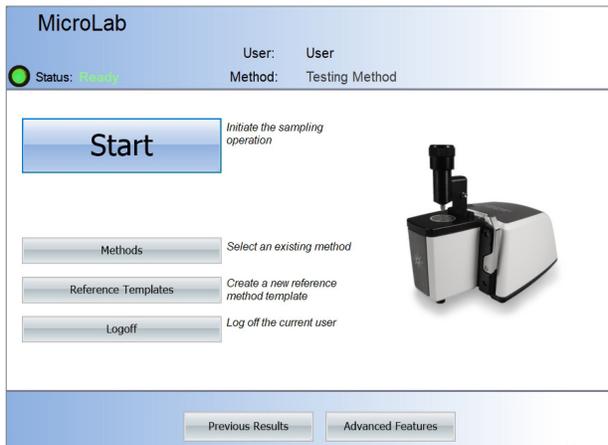
### Quantification



## Spectrum analysis



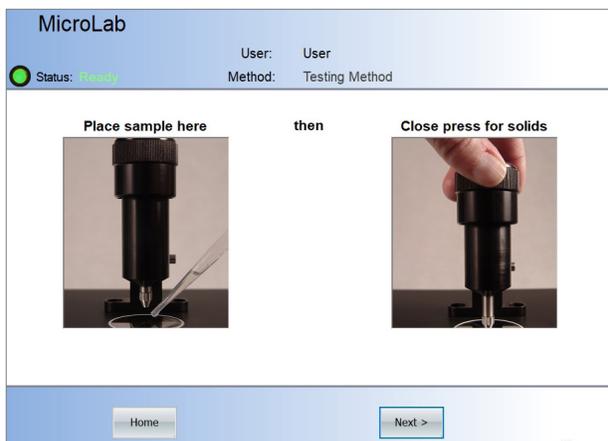
1 Start the analysis



A single click starts a picture-guided workflow that navigates the user through every step of the analysis. The software identifies the instrument and sampling interface in use and displays the relevant images.

After data collection, MicroLab performs all calculations and presents results that are easy to understand, even for novice users. MicroLab software provides color-coded results, which are reported directly after data acquisition, in line with the critical and marginal threshold settings of the method, as shown in Figure 1.

2 Follow picture-driven software guidance



3 Instantly receive color-coded, actionable results

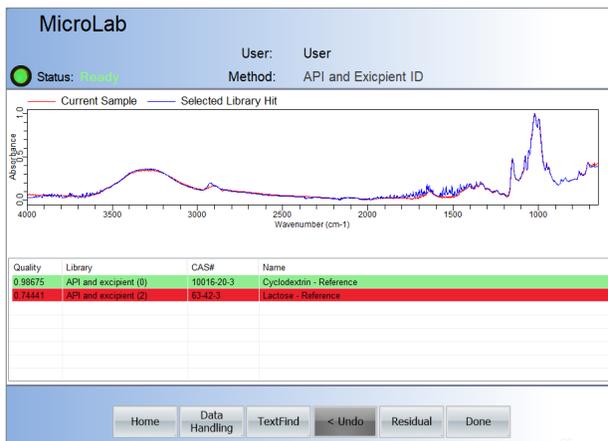
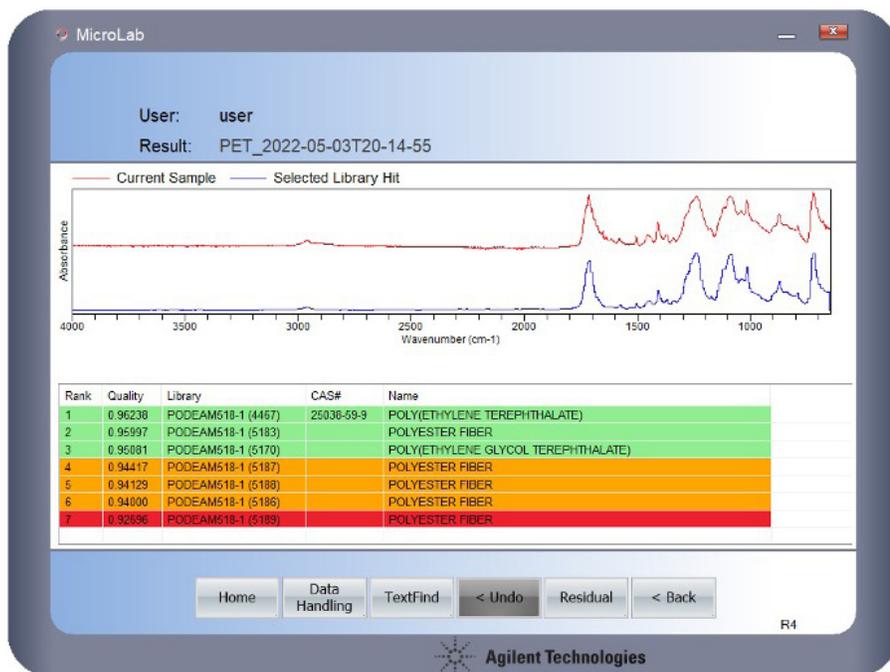


Figure 1. Three simple steps using Agilent MicroLab software and Agilent FTIR spectrometers that make performing an analysis straightforward, with reduced training needs.

### Identification applications

MicroLab automatically compares the collected spectrum with a spectral library and finds the best spectral match. For easy interpretation, color-coding can be applied based on confidence levels (Figure 2).



**Figure 2.** Confirm the identity of your sample by displaying high-quality matches to reference spectra.

### Libraries are easily employed in MicroLab software.

- Agilent provides ready-to-use, application-specific libraries.
- Users can create their own libraries in seconds.

### Library searches can be tailored to the identification application.

- Multiple libraries can be searched simultaneously, for example one library with reference standards to identify the sample, and another library with out-of-specification samples to identify re-occurring problems.
- A broad selection of search algorithms is available.
- Spectral ranges can be excluded from the analysis.
- Minimal high quality index (HQI) and maximum number of hits settings ensure only relevant library hits are presented.
- Color-coding of the results based on the HQI can be used to define confidence levels.

### Identification is simple with an easy-to-understand display of results.

### Examples of applications include:

- Quickly confirming the purity of incoming chemicals and final products.
- Using spectral libraries to quickly authenticate solvents, surfactants, specialty amines, or industrial organic chemicals.
- Identifying narcotic analogs in unknown seized samples.

## MicroLab PC and MicroLab Lite

For detection applications, relevant safety and hazard information is clearly displayed in all results windows (Figure 3). Further detailed information can be accessed, including the Custom Information section, which is editable by the user (Figure 4).

User: User  
Result: MDMA (G19-428)\_2022-04-11T12-10-12

Results:

| Warning | Rank | Quality | Library      | CAS#         | Name                                                   |
|---------|------|---------|--------------|--------------|--------------------------------------------------------|
| ⚠       | 1    | 0.98088 | TICTAC (157) | 42542-10-9   | Crystal MDMA                                           |
| ⚠       | 2    | 0.66617 | TICTAC (376) | 74341-78-9   | MDEA                                                   |
| ⚠       | 3    | 0.66412 | TICTAC (225) | 42542-10-9   | 3,4-methylenedioxyamphetamine                          |
| ⚠       | 4    | 0.57692 | TICTAC (18)  | 1134709-81-1 | 1-Methylamino-1-(3,4-methylenedioxyphenyl)-propane HCl |
| ⚠       | 5    | 0.49890 | TICTAC (3)   | 39512-50-0   | 1-(2-Chlorophenyl)-piperazine                          |
| ⚠       | 6    | 0.46246 | TICTAC (340) | 4764-17-4    | 3,4-Methylenedioxyamphetamine hydrochloride            |

**Rank 1**    **MDMA HCl**    **Sample Description**

42542-10-9    Controlled Substance    Commonly known as ecstasy (E), a psychoactive drug used primarily as a recreational drug.

⚠    ⚠    ⚠

More

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Agilent Technologies

**Figure 3.** Clear, actionable safety and hazard information for the selected library hit, including a CAS number, GHS symbols, a warning flag (for controlled substances), and a brief sample description.

**Identification**

Chemical Name: MDMA HCl  
Source Library: TICTAC  
IUPAC Name: 1-(1,3-benzodioxol-5-yl)-N-methylpropan-2-amine  
CAS#: 42542-10-9  
EC Number: Not Available  
Emergency Response Code: Not Available  
UN Number: Not Available

**MDMA HCl**

First Aid Measures: Not Available  
Firefighting Measures: Not Available  
Accidental Release Measures: SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

**Data**

Alternate Name: MDMA;3,4-methylenedioxyamphetamine;Ecstasy;Methylenedioxyamphetamine;DL-(3,4-methylenedioxy)methamphetamine;(RS)-3,4-(methylenedioxy)methamphetamine  
Sample Description: Commonly known as ecstasy (E), a psychoactive drug used primarily as a recreational drug.  
Molecular Formula: C<sub>11</sub>H<sub>15</sub>NO<sub>2</sub>  
Molecular Weight: 193.2423  
Concentration: Not Available  
Melting Point: Not Available  
Density: Not Available  
Flash Point: Not Available

**Custom Information**

Class: Not Available  
Notes: Not Available  
Handling: Not Available

< Back

**Figure 4.** Additional chemical and first-response information. The editable Custom Information section provides further user-specific guidance.

### Quantification applications

MicroLab allows users to quantify multiple components in a sample with a single FTIR measurement. Basic quantification models can be easily created in MicroLab Quant. For more comprehensive chemometric models, MicroLab also supports prediction models developed in MicroLab Expert.

- **With MicroLab's unique, logic-setting capabilities, only relevant results are displayed.**
- **User-defined criteria for color-coded results (red, yellow, green) provide great flexibility.**
- **MicroLab performs all calculations and instantly provides color-coded, actionable results and follow-up instructions.**

- **Examples of applications include:**
  - Ensuring manufacturer's specifications are met by accurately measuring levels of known additives.
  - Ensuring blends and mixtures of fine chemicals are properly formulated.
  - Obtaining fast, easy, and reliable measurements of liquid samples using transmission FTIR.

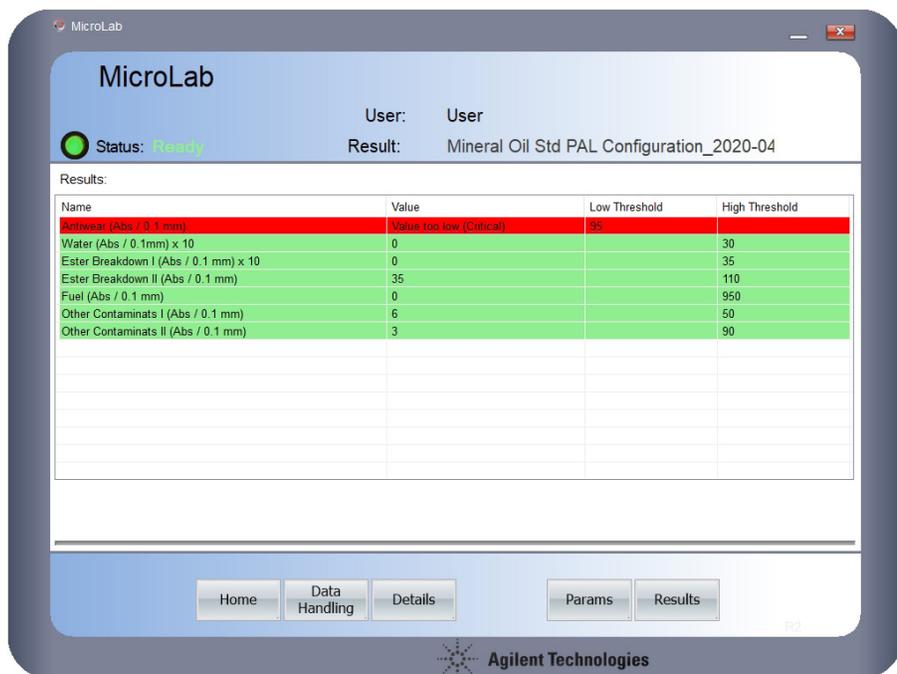


Figure 5. The MicroLab software automatically performs all calculations and displays the final result color-coded for easy review.

### Collect and review infrared spectra

MicroLab can also be used to collect and review an infrared (IR) spectrum of a sample. An IR spectrum can provide valuable insights such as the presence of functional groups.

- MicroLab allows users to change the wavenumber scaling factor for a more detailed analysis of the spectra range of interest.
- Bands can be labeled for reporting or comparison against literature values (Figure 6)



**Figure 6.** MicroLab software allows operators to collect, review, and re-analyze infrared spectra of samples, along with a reporting feature.

Report all your results

MicroLab PC and Lite incorporate predefined and customizable report templates. Results can be automatically reported, and a consistent format allows swift review of relevant details (Figure 7). Report templates can be edited in Microsoft Word.

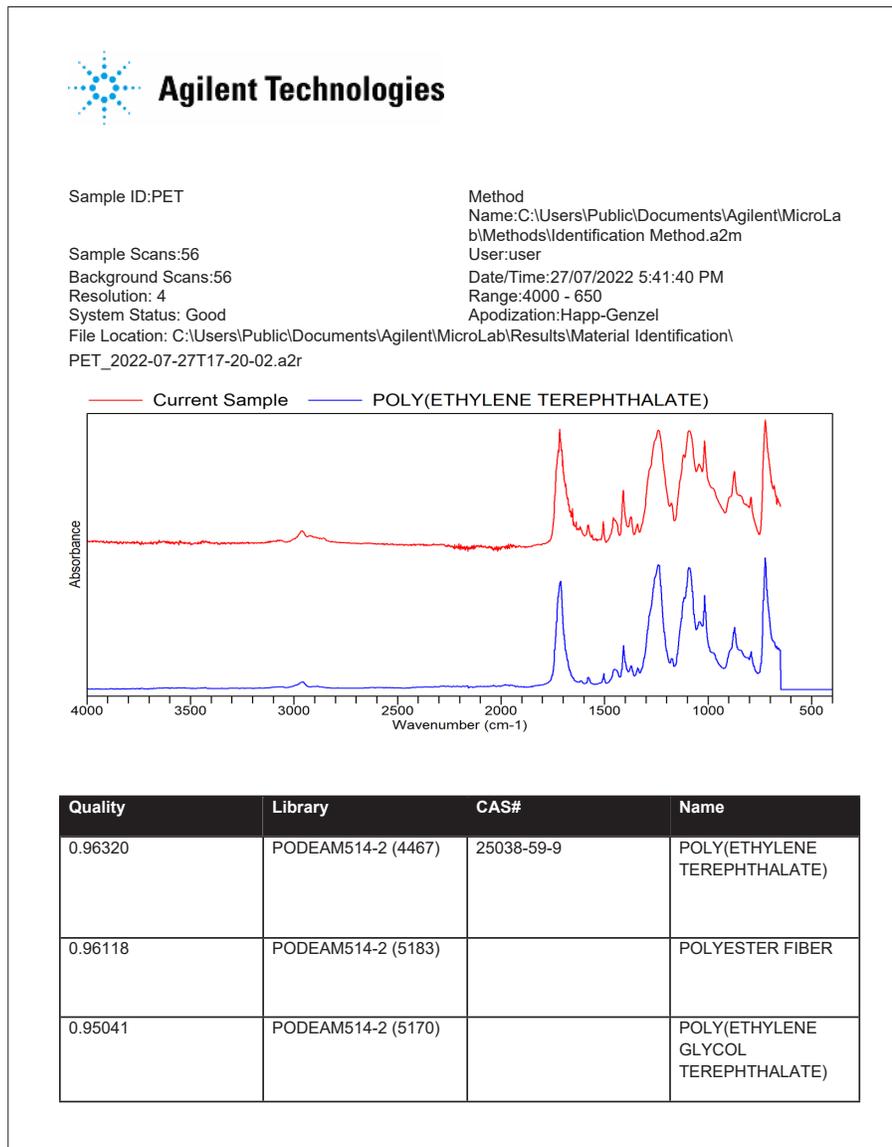
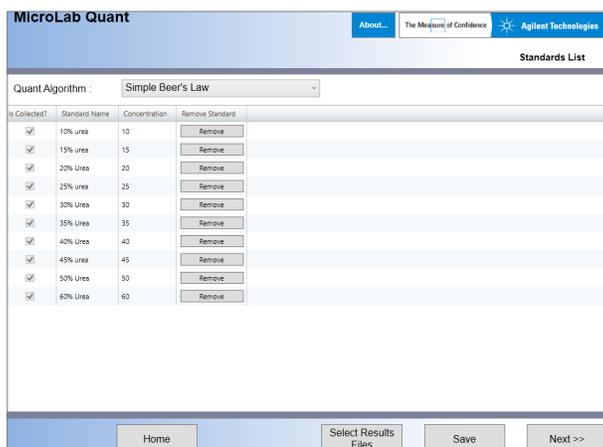


Figure 7. Results report generated using MicroLab software. All relevant details of the analyzed sample can be captured in the generated report for record keeping.

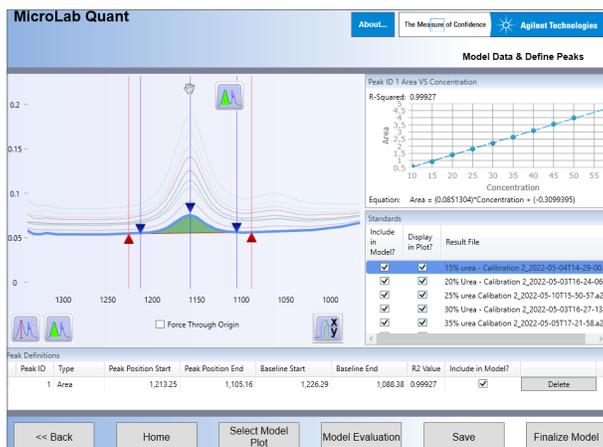
# MicroLab Quant

MicroLab Quant features the same step-by-step guidance as the rest of the MicroLab software suite and expands the fast and simple software experience to model development for quantitative applications (Figure 8). Seamless data integration allows the easy use of IR spectra and quantification models in MicroLab PC, MicroLab Lite, and MicroLab Quant.

## 1 Select standards and enter concentrations



## 2 Define peaks and optimize calibration



## 3 Finalize the model and use it in MicroLab

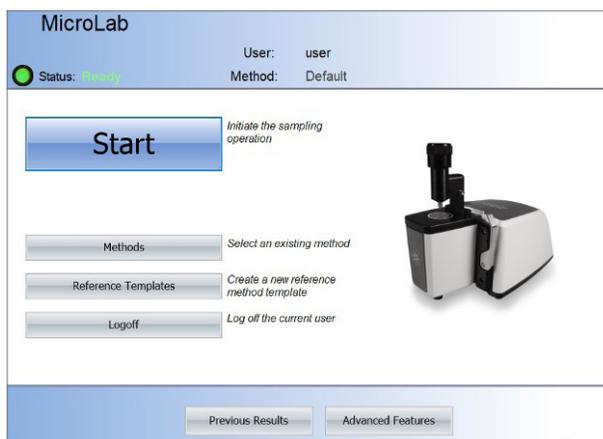


Figure 8. Easy steps of MicroLab Quant software to develop quantitative models.

## MicroLab Quant

- The interactive software interface allows swift and easy creation and optimization of quant models (Figure 9).
- Direct feedback shows the influence of any change to the correlation graph.
- Quantification models can be evaluated with cross or independent sample validation (Figure 10).

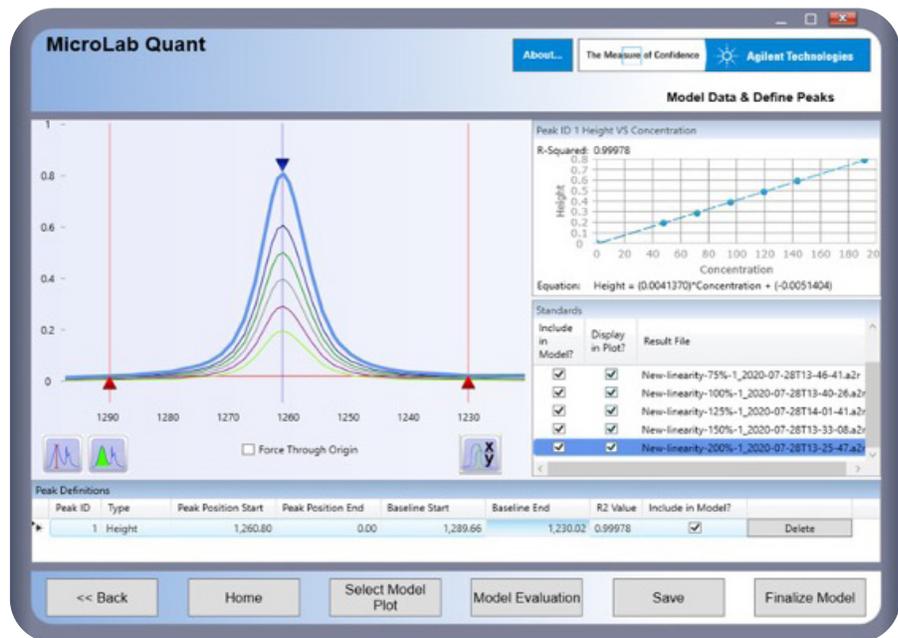


Figure 9. Linearity evaluation of the DialPath sampling module using MicroLab Quant. Calibration curves and correlation coefficient calculations are performed automatically in the software.

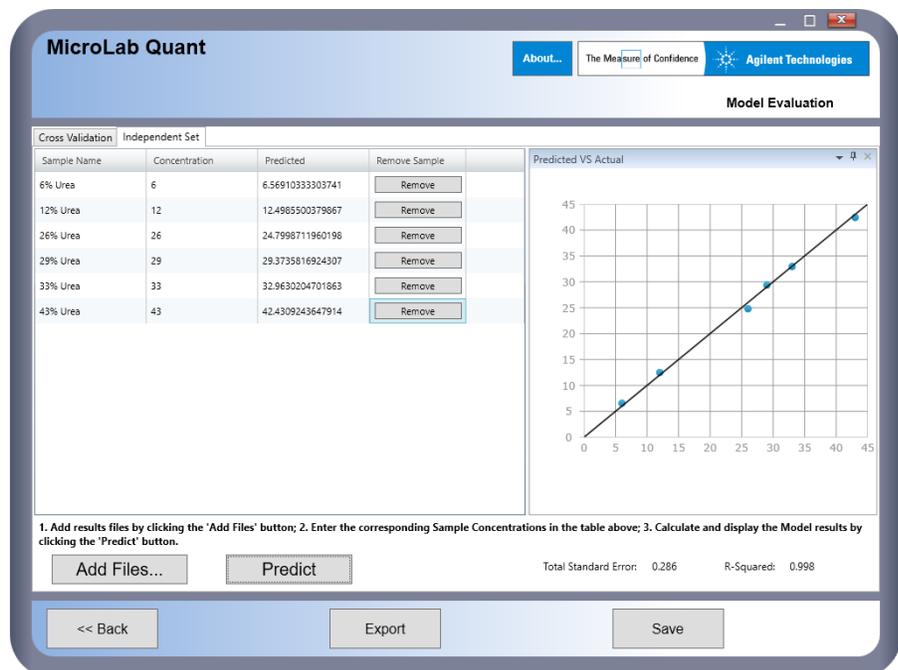


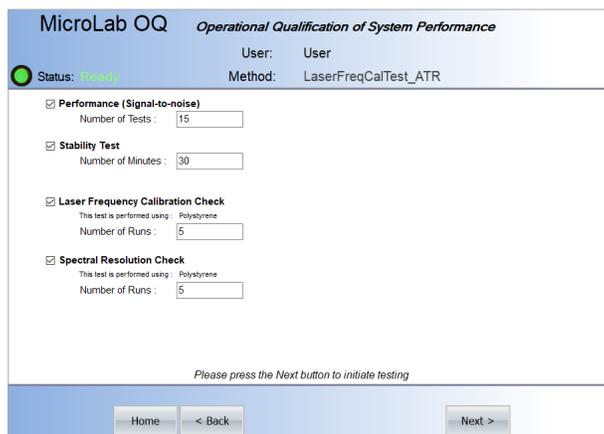
Figure 10. The MicroLab Quant application also allows users to evaluate the developed quantification modules, either through cross validation, or against a separate sample set.

# MicroLab OQ

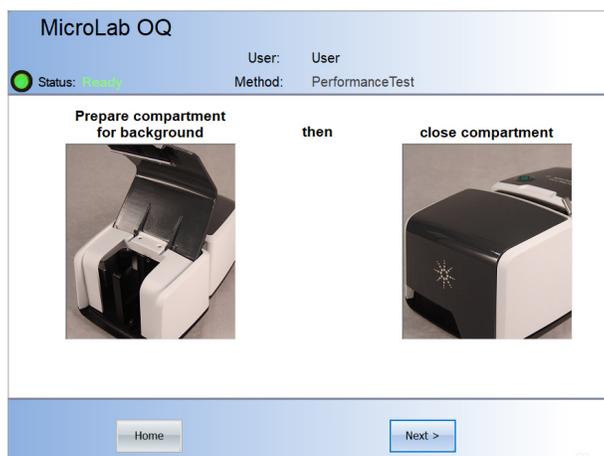
Control of instrument performance is a critical aspect in qualifying an instrument's suitability for the intended analysis. MicroLab OQ allows users to easily perform instrument performance checks to ensure that an instrument is in good condition.

MicroLab OQ has an intuitive, pictorial interface, which guides users through the qualification process.

## 1 Select instrument performance tests



## 2 MicroLab OQ guides through each test



## 3 Review performance test summary

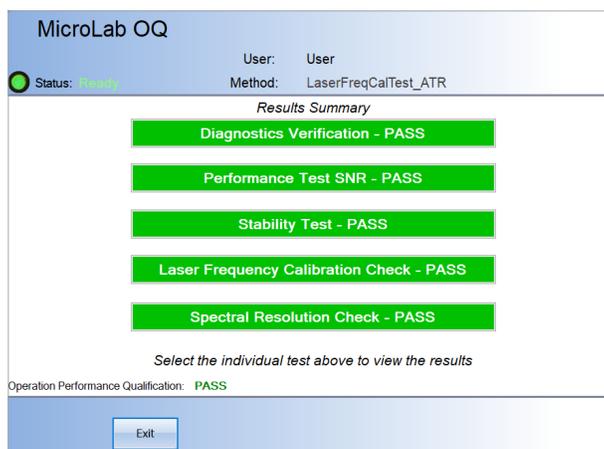
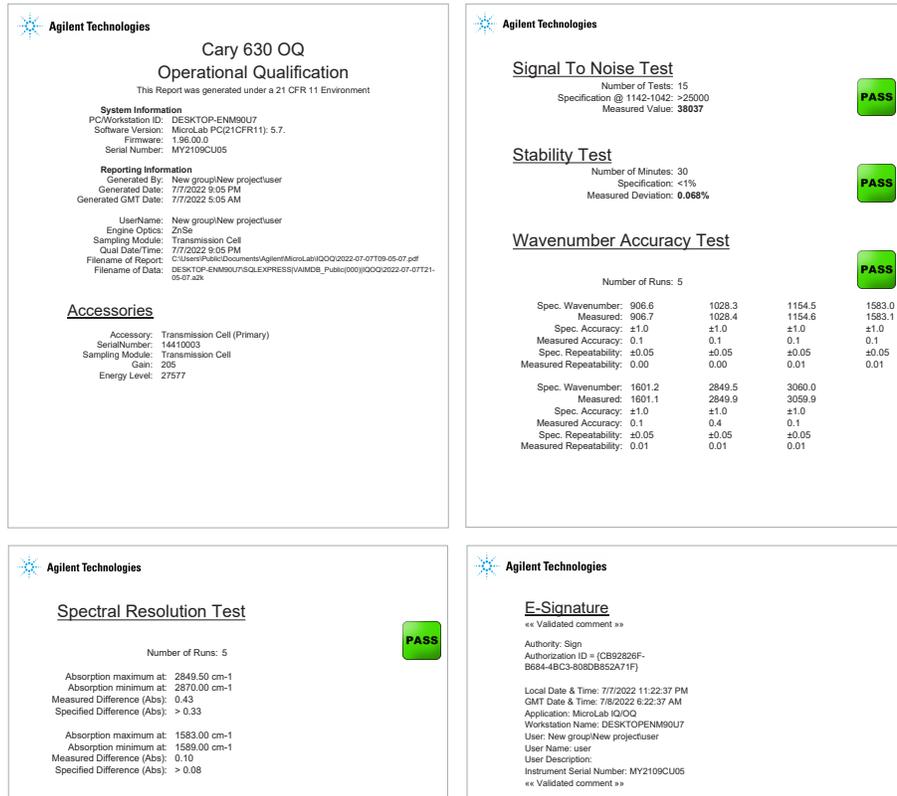


Figure 11. MicroLab OQ guides users to perform instrument qualification through simple and easy steps.

# MicroLab OQ

On the last step, MicroLab OQ generates a PDF report showing the diagnostic values, the test results, and the specifications for the tests and pass/fail criteria for future reference (Figure 12).



**Figure 12.** Operational Qualification (OQ) report generated using MicroLab OQ. Results are reported with all test parameters along with easy-to-read pass/fail results.

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