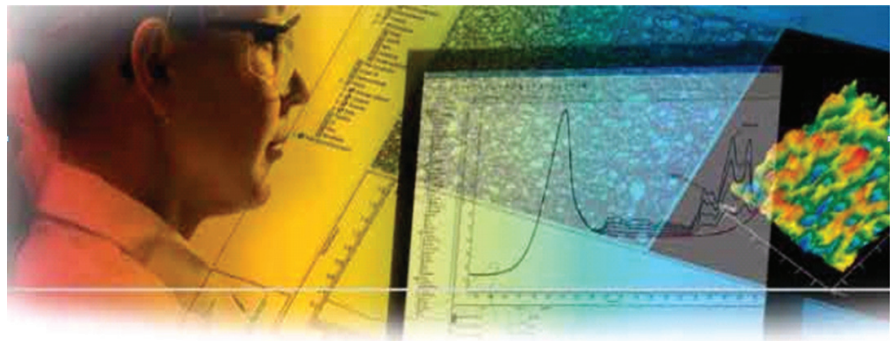# MicroLab FTIR Software

Technical Overview

Introduction

The Agilent Cary 630 FTIR provides a robust, easy-to-use, superior performing FTIR in a compact package. In part, what makes the Cary 630 FTIR unique is the software package or interface that accompanies it. Agilent MicroLab FTIR software allows users of all levels to use it for applications from unknown material identification and characterization to detailed quantitative analysis.

Agilent Technologies

Ease-of-use

MicroLab FTIR software uses a methods-based platform to make the software walk-up friendly. The administrator can choose which methods are available to the technician or end user. They simply walk up, select the method and begin by clicking the 'Start' button. From here, the software guides the user based on the accessory or sampling interface in how to introduce the sample and take a measurement (Figure 1). This allows even a novice user to be able to instantly take accurate and reproducible measurements.
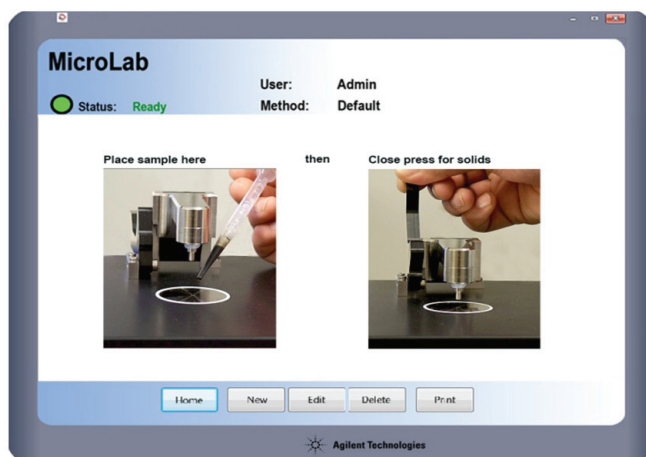

Figure 1. Intuitive MicroLab FTIR software guides users through steps

Qualitative and quantitative results in one package

MicroLab FTIR software offers easy qualitative and quantitative analysis. The method-driven design takes users from sample measurement through to the desired results, guiding them the entire way to ensure proper technique and accurate results. The method editor allows users to easily set up either qualitative, library search methods or quantitative methods. Methods contain all needed information from data collection parameters to quantitative calibrations or library search parameters. Once established, these methods make it simple for users to make accurate measurements time after time.

Library search methods allow the data to be searched against multiple libraries, either user-generated or commercial. The administrator can choose to limit the search results, such that only results with a selected correlation are shown. The 'Details' button shows a comparison between the collected data and the library spectra; the display can be stacked or overlaid for easy visual comparison (Figure 2).
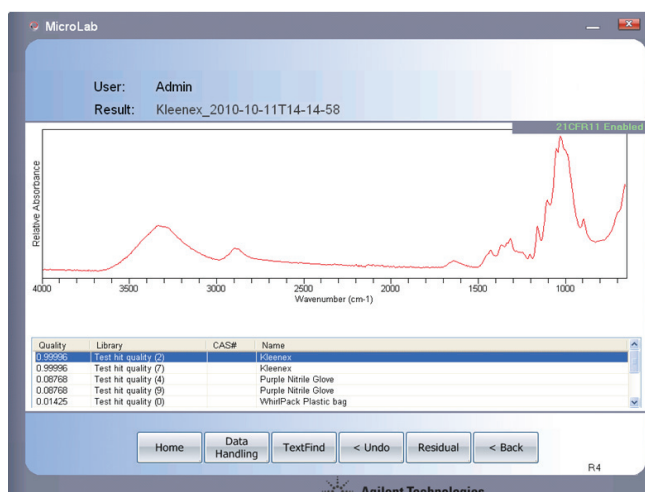

Figure 2. Identify unknowns by comparison with library spectra

Quantitative measurements, called Component Methods, are also easy with the MicroLab FTIR software. Once the methods are established, the software takes the user from sample measurement directly to the quantitative results. The MicroLab method wizard allows for linear or multivariate calibrations. Linear calibrations can be made using all common peak measurement tools (area, height, baseline correction, ratio and band center). Multivariate (PLS, PCR, and so forth) calibrations are performed in a powerful third party software then transferred directly to the MicroLab software. Quantitative measurement of multiple analytes can be configured within a single method. By directly attaching the quantitative analysis to the component method, MicroLab ensures that the correct results are obtained every time.

Visual results

Part of MicroLab FTIR's easy-to-use features is simple to understand results. In addition to taking the user directly to the quantitative or search results, the results can be color-coded to indicate where the sample falls with respect to a specification. Marginal and critical levels can be set in component methods to show the result as yellow or red respectively, making the results clear to the user. Numeric results can also be replaced with text, such as 'PASS' or 'FAIL', making the answers even easier for untrained users (Figure 3).
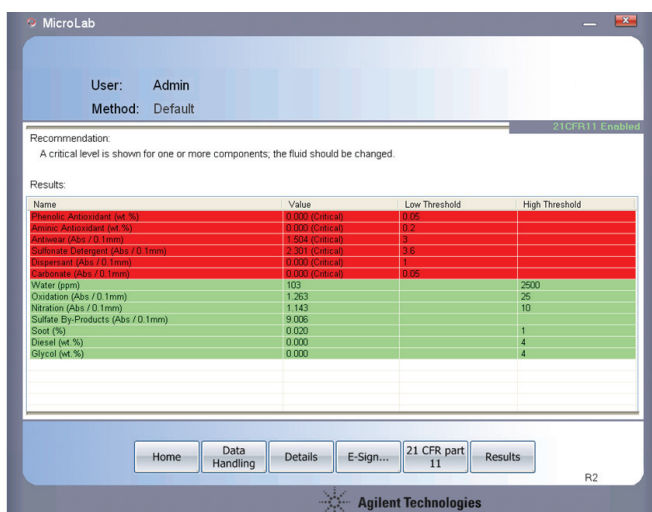

Figure 3. Easily interpret quantitative results with conditional reporting

Additionally, MicroLab FTIR allows the method developer to set reporting criteria for any component in the method; reporting criteria can be based on predicted concentrations or statistical values generated from a multivariate analysis. One use of this component reporting feature is two calibrations to cover a wide dynamic range of analyte concentrations; the component reporting feature can be used to only display the concentration result from the appropriate calibration. This further serves to guarantee correct results with little user input.

GLP/GMP compliance

MicroLab FTIR software provides an easy-to-use interface for simple to complex applications, all the while ensuring that you meet the requirements within your lab for GLP/GMP compliance. The base software allows for user level control and password protection within the software, ensuring that the software is only initialized by those with the appropriate access. The user level access also allows the administrator to determine which methods the Technician level can access. Only methods designated as 'Public' can be used by all users (Figure 4).
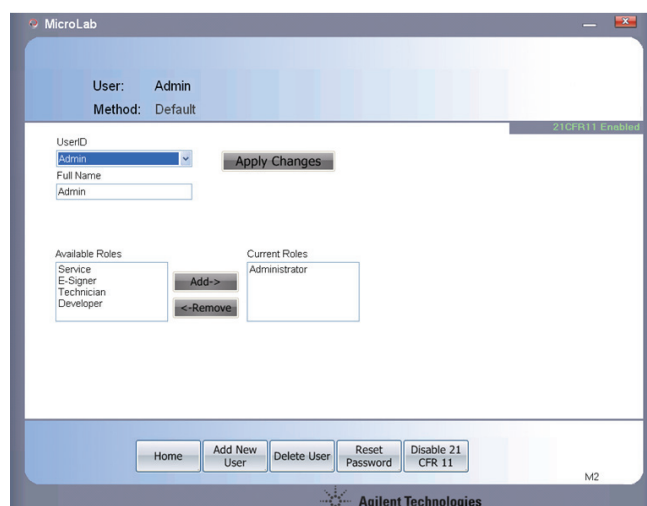

Figure 4. Securely maintain user access

Summary

Powerful MicroLab FTIR software ensures that you get the answers you need quickly. It guides users pictorially from sample introduction to analysis for both qualitative and quantitative measurements.

www.agilent.com/chem

Agilent shall not be liable for errors contained herein or for incidental or consequential damages in connection with the furnishing, performance or use of this material.

Information, descriptions, and specifications in this publication are subject to change without notice.

Agilent Technologies