

Automating standard operating procedures using simple scripting

Technical Overview

Advantage statement

Easy to create, customized software scripts created using Resolutions Pro Software reduce user training time and increase analysis speed, for increased productivity. The automated scripting steps reduce the chance of errors, increasing confidence in results.

Introduction

Scripting is a powerful tool that can automate a series of common steps. It is a software program within Agilent's Resolutions Pro that transforms a Fourier transform infrared (FTIR) spectrometer into a dedicated analyzer in minutes. Scripting does NOT involve computer programming; rather a user need only put together a desired list of actions to be performed. The software guides a user through 'one-click' dialogue boxes from start to finish, thereby allowing novice users to obtain high-quality data in seconds and drastically reducing chances of errors. Scripting is an ideal tool for routine QA/QC applications as it can provide both qualitative and quantitative information without the analyst having to interpret (or even understand) the results. A scripting routine can be used to automatically perform all spectral collection and processing steps, and if desired, can automatically print a customized report. Advantageously, scripting can be performed in any language.

There are four principle actions to be performed in order to create and run a simple script. These steps include: (I) Establishing a method (that is, define the number of co-added scans, spectral resolution), (II) Choosing post-spectral collection processing to be applied (that is, peak picking, spectral searching against a database, printing of a customized report), (III) Adding a customized method and prompts to a script, and (IV) Running the script.



This advantage note provides an illustrated step-by-step example of simple scripting within the Resolutions Pro software. It highlights the simplicity in both creating and running a script for routine analyses using an attenuated total reflectance (ATR) accessory.

Establishing a Method

A collection method allows you to input a basic set of collection parameters (tailored to your Standard Operating Procedures) such as an appropriate number of co-added scans for the sample and background as well as the spectral resolution. You can use a default collection method within Resolutions Pro which can be found in the Method Editor dialog box.

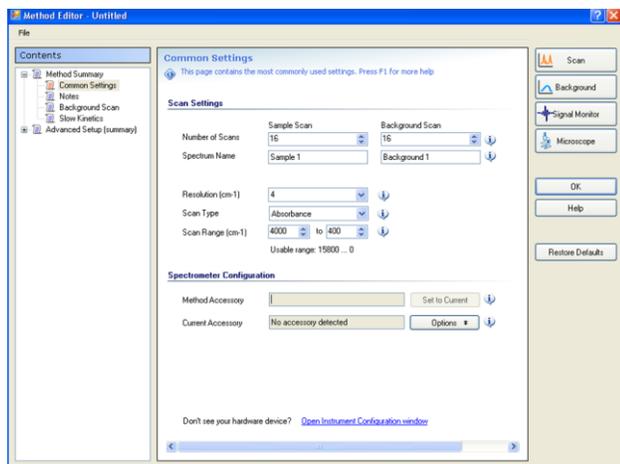


Figure 1. Method Editor dialog box in Resolutions Pro

The next step is to ensure that a clean ATR accessory is properly inserted into a Cary 600 FTIR spectrometer's sample compartment.



Figure 2. Cary 640 FTIR spectrometer with ATR fitted

Post-Spectral Collection Processing

Selecting and applying post-spectral collection processing to be included in a scripting routine can be done in minutes and will result in tremendous time-savings. Common processing includes peak labeling using the Peak Pick feature (Figure 3), spectral searching against a database (commercially-available or in-house) using the Search feature for improved identification of unknowns (Figure 4), and printing a customized report using the Print Composition feature (Figure 5).

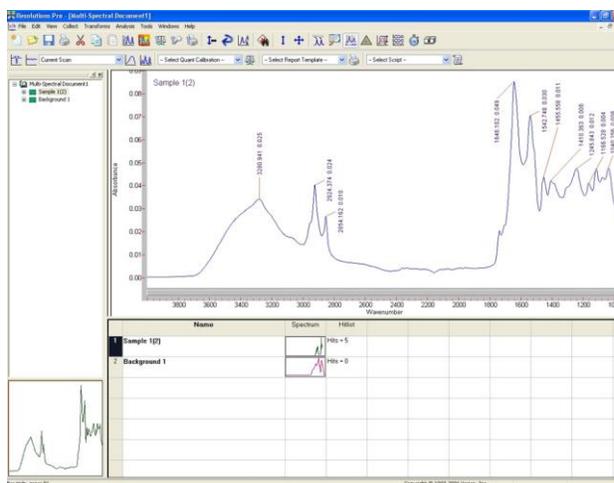


Figure 3. Peaks are automatically labeled and tabulated using the Peak Pick feature

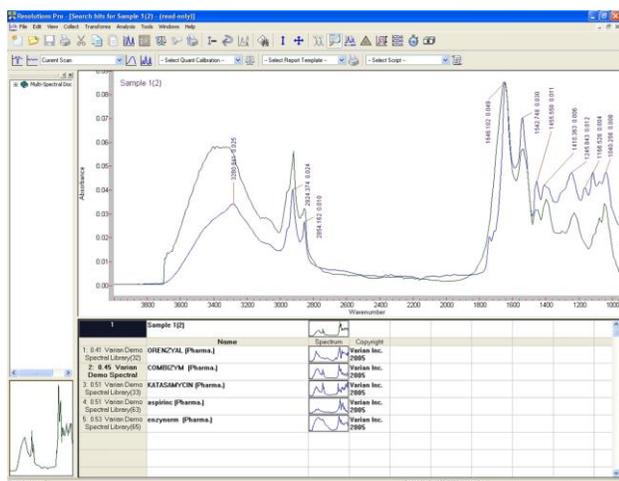


Figure 4. Agilent’s spectral search can be used for databases constructed in-house

Adding a customized method and prompts to a script

The EditSimon feature affords users the flexibility to create a script with a user-defined number of steps (depending on the user’s experience level). Prompts can be written in any language and are readily customized to suit any protocol. A number of common prompts are provided as an illustrative example of the capabilities of scripting in the next section.

Running the script

A script can be initiated from a drop-down menu on Resolutions Pro Software’s main interface. All that remains is to follow the on-screen instructions that are a series of ‘one click’ buttons as illustrated below (Figure 6). The operator need only have a very basic understanding of FTIR spectroscopy to extract high quality data.

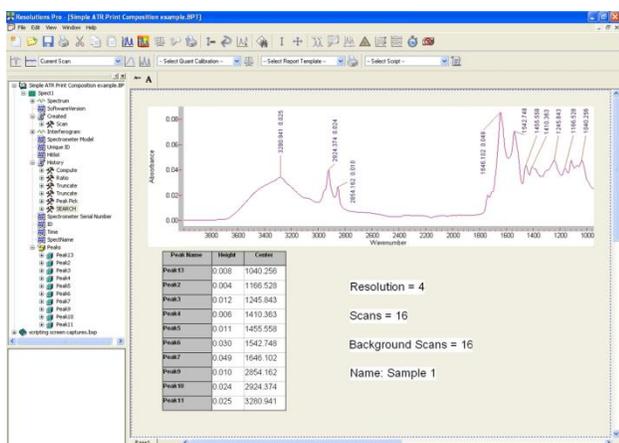


Figure 5. The Print Composition feature allows a user to create a standardized (customized) report for improved traceability

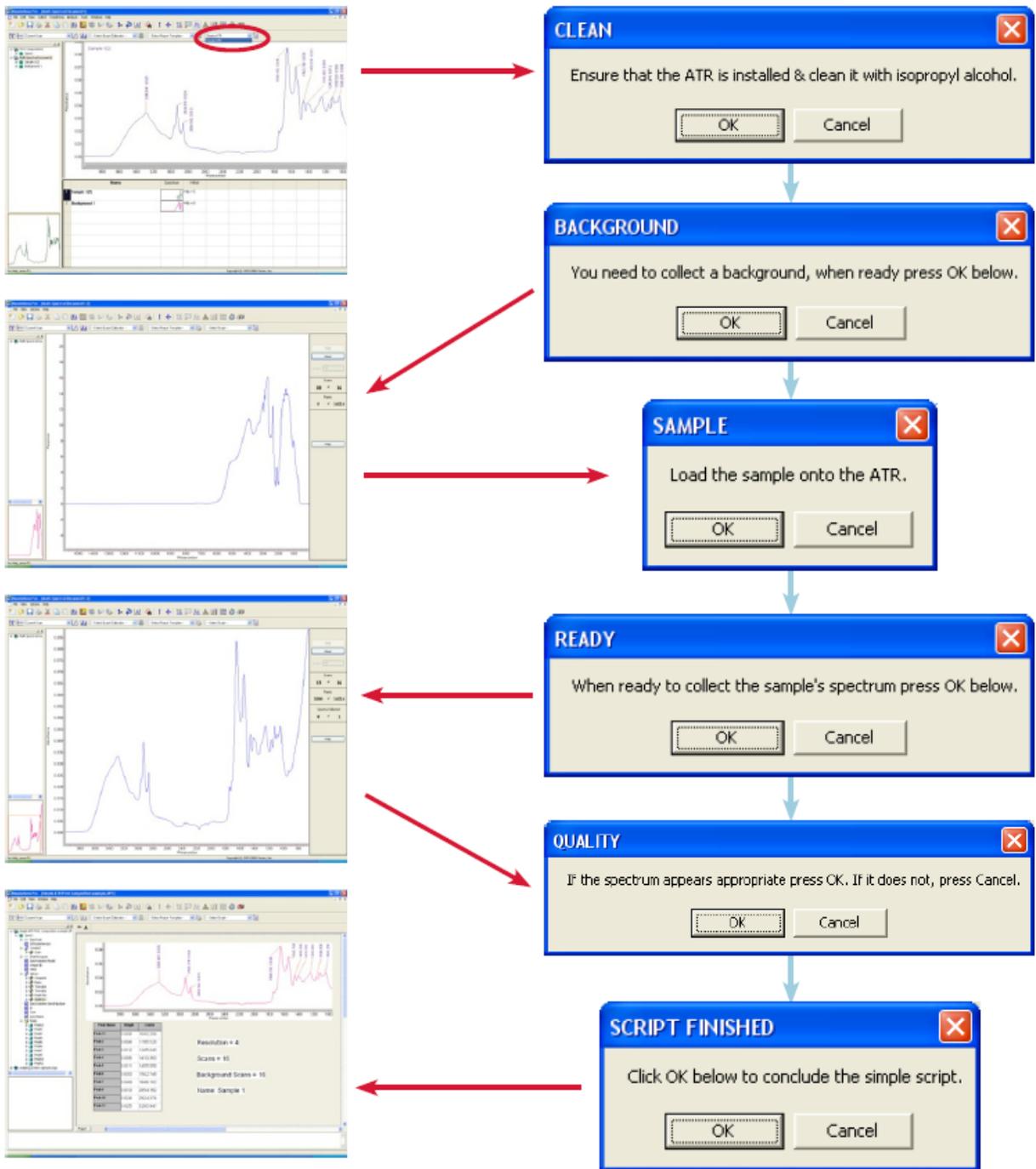


Figure 6. Automation of a standard operating procedure allows for high-quality spectra to be collected in seconds by novice users, reduces chances for protocol deviations and provides customizable printed reports that include advanced data interpretation

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