Agilent

Instrument Qualification of the Cary 630 FTIR in accordance with Japanese Pharmacopeia (JP)

Instruction Sheet

Contents

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1 Scope

This method development guide aims to assist users in qualifying their instruments following the standards outlined in the Japanese Pharmacopeia (JP). It provides comprehensive guidance on the method development process, encompassing the establishment and utilization of three routine MicroLab methods. The JP defines instrument qualification for infrared spectrophotometry in chapter 2.25. For an FTIR instrument to be qualified in accordance with the JP, Wave Number Scale (equivalent to wavenumber accuracy) and Resolving Power (equivalent to spectral resolution) must be verified. Additionally, the JP specifies two additional parameters that must be verified: Transmittance Reproducibility and Wave Number Reproducibility. Test descriptions and test limits can be found in Table 1.

Table 1 JP system verification test descriptions and test limits.

Test description	Acceptable threshold	
Wave Number Scale		
Position of band maxima of polystyrene film	1028.3 cm^{-1} 1154.5 cm^{-1} 1583.0 cm^{-1} 1601.2 cm^{-1} (1942.9 cm^{-1})(1) 2849.5 cm^{-1} 3060.0 cm^{-1}	±1.0 cm^{-1} ±1.0 cm^{-1} ±1.0 cm^{-1} ±1.0 cm^{-1} ±1.5 cm^{-1} ±1.5 cm^{-1} ±1.5 cm^{-1}
Resolving Power		
The depth of the trough from the maximum absorption at about 2850 cm^{-1} to the minimum at about 2870 cm^{-1}	≥18% transmittance	
The depth of the trough from the maximum at about 1583 cm^{-1} to the minimum at about 1589 cm^{-1}	≥12% transmittance	
Wave Number Reproducibility		
Difference of wavenumber of two spectra at about 3060 cm^{-1}	<5 cm^{-1}	
Difference of wavenumber of two spectra at about 1028 cm^{-1}	<1 cm^{-1}	
Transmittance Reproducibility		
Difference of transmittance of several bands measured twice from 3000 to 1000 cm^{-1} at: • about 3060 cm^{-1} • about 2849 cm^{-1} • about 1601 cm^{-1} • about 1583 cm^{-1} • about 1154 cm^{-1} • about 1028 cm^{-1}	<0.5%	

(1) The band at around 1942.9 cm^{-1} was determined in NIST SRM 1921b by "extrapolated center of gravity". MicroLab uses "center of gravity" peak determination. It is therefore justifiable that this setpoint is omitted from the Wave Number Scale test without compromising the qualification requirements. For details, please contact your local Agilent representative.

Scope

This document describes the following procedures:

- Chapter 2: Equipment and Material
- Chapter 3: Generation of three individual methods in the Agilent MicroLab software to verify:
  - Wave Number Scale
  - Resolving Power
  - Transmittance Reproducibility and Wave Number Reproducibility
- Chapter 4: Generation of report templates for the three methods
- Chapter 5: Execution of the three methods using the Cary 630 FTIR

2 Equipment and Materials

The following equipment and materials are required for the method development following this application guide.

2.1 Materials

The use of a NIST SRM 1921b traceable polystyrene film of approximately 35 µm thickness is recommended (available from Agilent: p/n: 925-0128).

2.2 Instrumentation

- Agilent Cary 630 FTIR spectrometer with transmission sampling module
- Agilent MicroLab software

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3 Method Development

3.1 Create a method for the Wave Number Scale

Create a copy of the "LaserFreqCalTest_Transmission" method

1 Start MicroLab PC or MicroLab Lite.

2 Click Methods.

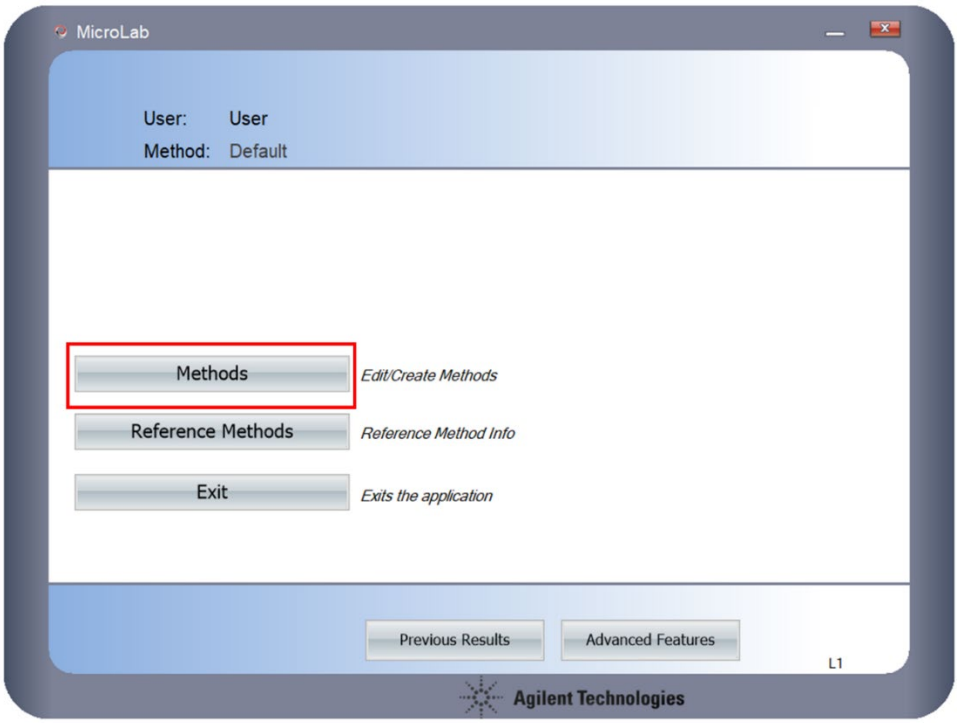

Figure 1. Methods button highlighted with a red rectangle in the MicroLab interface

3 Select the "LaserFreqCalTest_Transmission" method.

4 Click Edit.

5 Click Save As... and save the method with a descriptive file name. We used "JP – WAVE NUMBER SCALE" for this example.

6 Select the created method and click Edit method.

Setup the components tab

1 Click the Components tab.

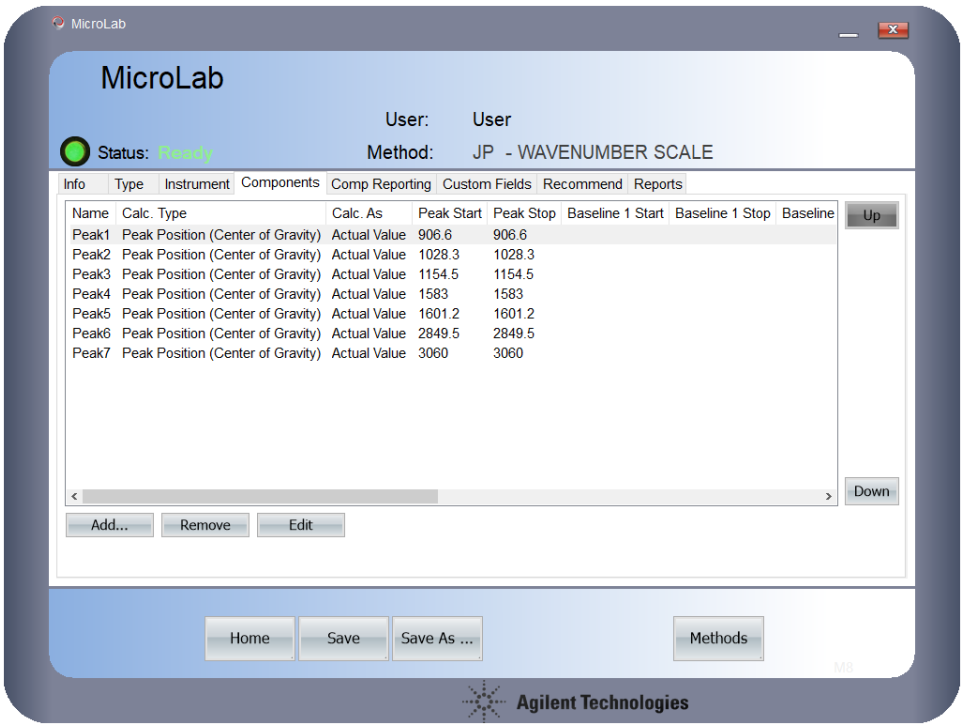

Figure 2. Peak 1 selected in the components tab of the MicroLab software

2 Select the component named “Peak1” and click **Remove**.

3 Select the component named “Peak2” and click **Edit.**

4 Change the **Component Name** to “Peak Position 1028.3”.

5 Change the **Decimal Digits To Report** to “1”.

6 In the **Thresholds** subsection set **Critical Low** to “1027.3” and **Critical High** to “1029.4”.

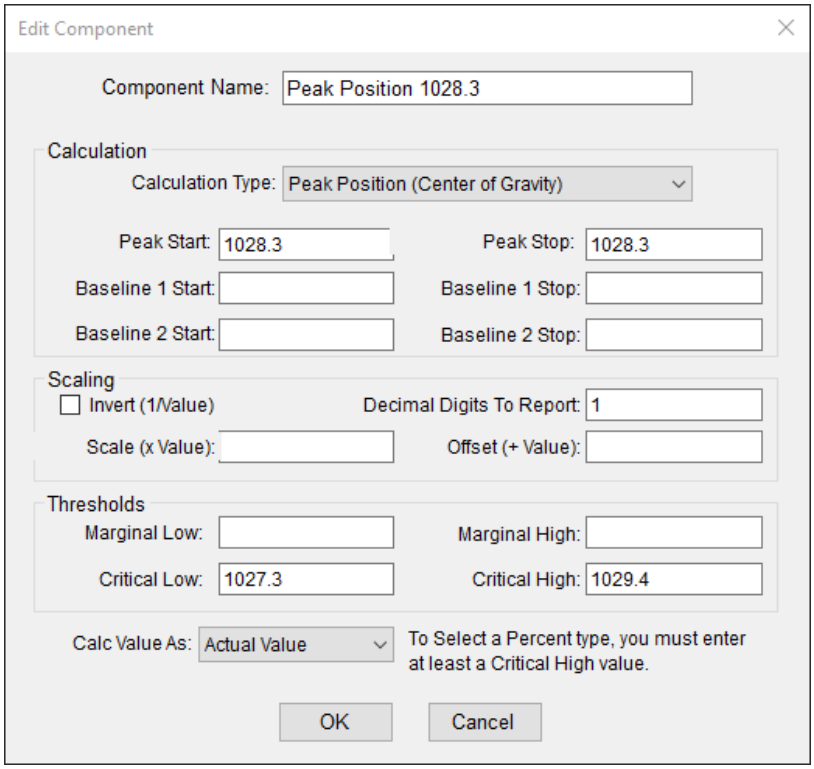

Figure 3. Threshold parameters

7 Click **OK**.

Repeat above steps **3** to **7** with for “Peak3” to “Peak7” with the details given in Table 2.

Table 2 Component parameters for Peak3 to Peak7

Old component name	New component name	Decimal Digits To Report	Thresholds	
			Critical Low	Critical High
Peak 3	“Peak Position 1154.5”	1	1153.5	1155.6
Peak 4	“Peak Position 1583”	1	1582	1584.1
Peak 5	“Peak Position 1601.2”	1	1600.2	1602.3
Peak 6	“Peak Position 2849.5”	1	2848	2851.1
Peak 7	“Peak Position 3060”	1	3058.5	3061.6

8 Click **Add**.

9 Set up the component with the following parameters:

Component Name: “Acc. Peak 1028.3.”

Calculation: Select Peak Position (Center of Gravity).

Peak Start: “1028.3”.

Peak Stop: “1028.3”.

Decimal Digits To Report: “1”.

Offset (+ Value): “-1028.3”.

Critical Low: “-1”.

Critical High: “1.1”.

10 Click **OK**.

11 Repeat steps 8 to 10 with the details given in Table 3.

Table 3 Component parameters for various Acc. Peaks

Component Name	Calculation	Peak Start	Peak Stop	Decimal Digits To Report	Offset (+ Value	Critical Low	Critical High
“Acc. Peak 1154.5”	Peak Position (Center of Gravity)	1154.5	1154.5	1	-1154.5	-1	1.1
“Acc. Peak 1583”	Peak Position (Center of Gravity)	1583	1583	1	-1583	-1	1.1
“Acc. Peak 1601.2”	Peak Position (Center of Gravity)	1601.2	1601.2	1	-1601.2	-1	1.1
“Acc. Peak 2849.5”	Peak Position (Center of Gravity)	2849.5	2849.5	1	-2849.5	-1.5	1.6
“Acc. Peak 3060”	Peak Position (Center of Gravity)	3060	3060	1	-3060	-1.5	1.6

12 Click **Add**.

13 Set up the component with the following parameters:

Component Name: "Overall test result Positive".

Calculation: Select Peak Position (Center of Gravity).

Peak Start: "3060".

Peak Stop: "3060".

Decimal Digits To Report: "0".

Offset (+ Value): "1000000".

Critical Low: "1".

14 Click OK.

15 Click Add.

16 Set up the component with the following parameters:

Component Name: "Overall test result Negative".

Calculation: Select Peak Position (Center of Gravity).

Peak Start: "3060".

Peak Stop: "3060".

Decimal Digits To Report: "0".

Offset (+ Value): "1000000".

Critical High: "1".

17 Click OK.

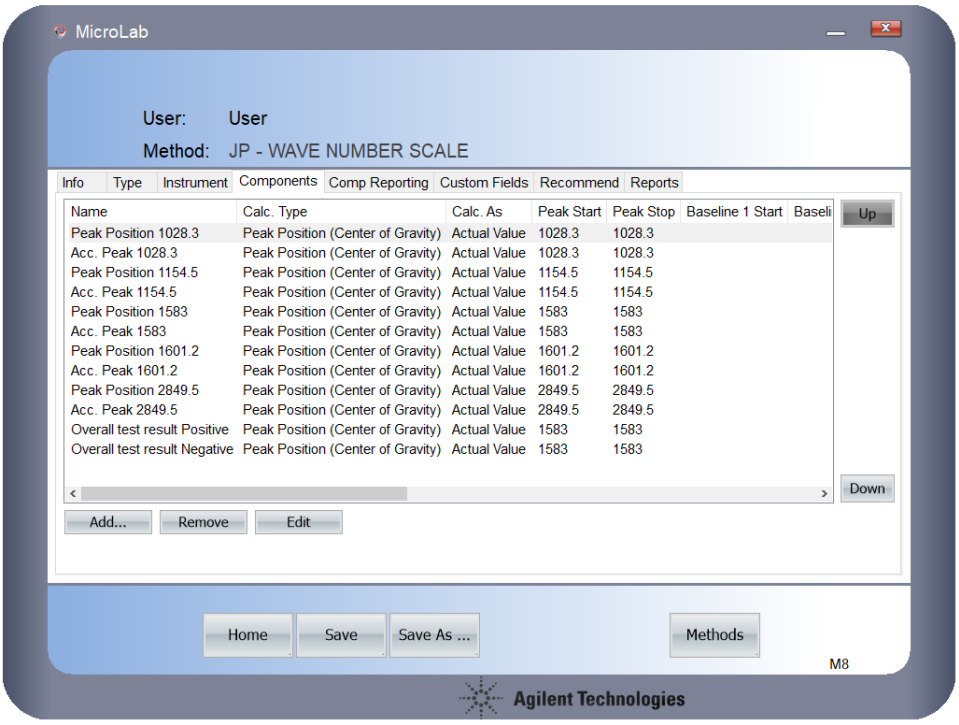

Figure 4. Components tab

Setup the component reporting

1 Click the **Comp Reporting** tab.

2 Select the component named “Peak Position 1028.3”.

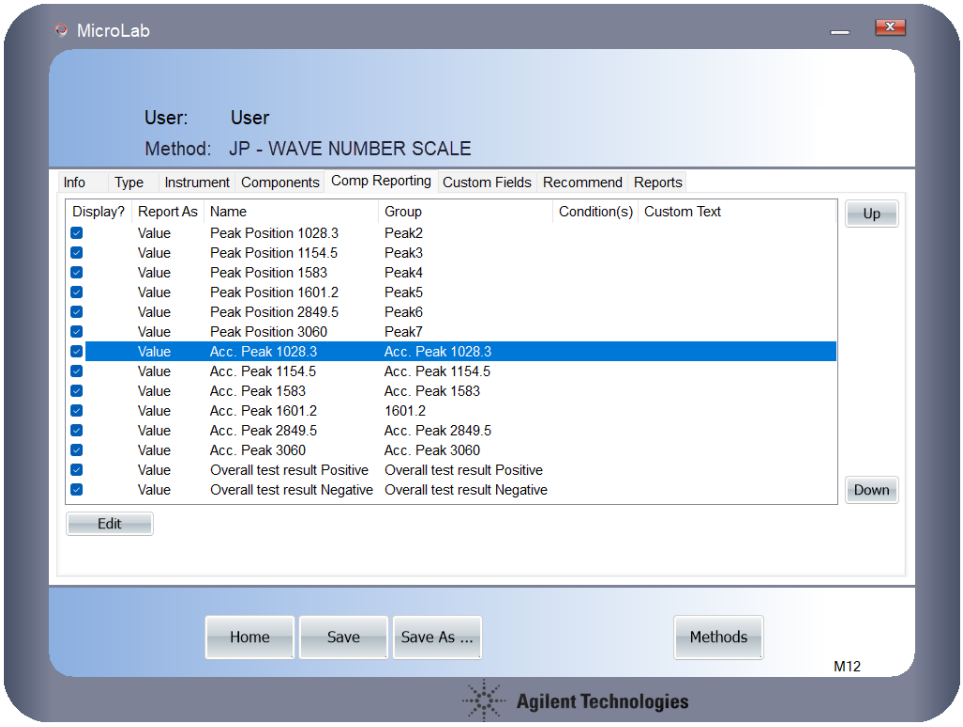

Figure 5. Component “Acc. Peak 1028.3” selected

3 Click **Edit.**

4 Change the **Group** to “Measured Peak Position (Spec. WN: 1028.3 cm^{-1})”.

5 Click **OK.**

6 Repeat steps 2 to 5 with the details given in Table 4.

Table 4 New group names for the peak positions

Component Name	New Group Name
“Peak Position 1154.5”	“Measured Peak Position (Spec. WN: 1154.5 cm^{-1})”
“Peak Position 1583”	“Measured Peak Position (Spec. WN: 1583 cm^{-1})”
“Peak Position 1601.2”	“Measured Peak Position (Spec. WN: 1601.2 cm^{-1})”
“Peak Position 2849.5”	“Measured Peak Position (Spec. WN: 2849.5 cm^{-1})”
“Peak Position 3060”	“Measured Peak Position (Spec. WN: 3060 cm^{-1})”

7 Select the component named “Acc. Peak 1028.3”.

8 Click **Edit**.

9 Change the **Group** to “Measured Accuracy (Peak at 1028.3 cm^{-1}, Spec. Acc.: +-1 cm^{-1})”.

10 Click **OK**.

11 Repeat steps 7 to 10 with the details given in Table 5.

Table 5 New group names for Acc. Peaks

Component Name	New Group Name
"Acc. Peak 1154.5"	"Measured Accuracy (Peak at 1154.5 cm^{-1}, Spec. Acc.: +-1 cm^{-1})"
"Acc. Peak 1583"	"Measured Accuracy (Peak at 1583 cm^{-1}, Spec. Acc.: +-1 cm^{-1})"
"Acc. Peak 1601.2"	"Measured Accuracy (Peak at 1601.2 cm^{-1}, Spec. Acc.: +-1 cm^{-1})"
"Acc. Peak 2849.5"	"Measured Accuracy (Peak at 2849.5 cm^{-1}, Spec. Acc.: +-1.5 cm^{-1})"
"Acc. Peak 3060"	"Measured Accuracy (Peak at 3060 cm^{-1}, Spec. Acc.: +-1.5 cm^{-1})"

12 Select the component named "Overall test result Positive".

13 Click **Edit**.

14 Change the **Group** to "Overall Test Result".

15 Change **Report As** to "Custom Text" and enter "PASS".

16 Set the **Component / Diagnostic Test** to "Peak Position 1028.3" and click **Add**.

17 Click **AND**.

18 Repeat steps 12 to 17 to set the "Condition" as:

"Peak Position 1028.3" is Good AND

"Acc. Peak 1028.3" is Good AND

"Peak Position 1154.5" is Good AND

"Acc. Peak 1154.5" is Good AND

"Peak Position 1583" is Good AND

"Acc. Peak 1583" is Good AND

"Peak Position 1601.2" is Good AND

"Acc. Peak 1601.2" is Good AND

"Peak Position 2849" is Good AND

"Acc. Peak 2849.5" is Good AND

"Peak Position 3060" is Good AND

"Acc. Peak 3060" is Good AND

19 Click **OK.**

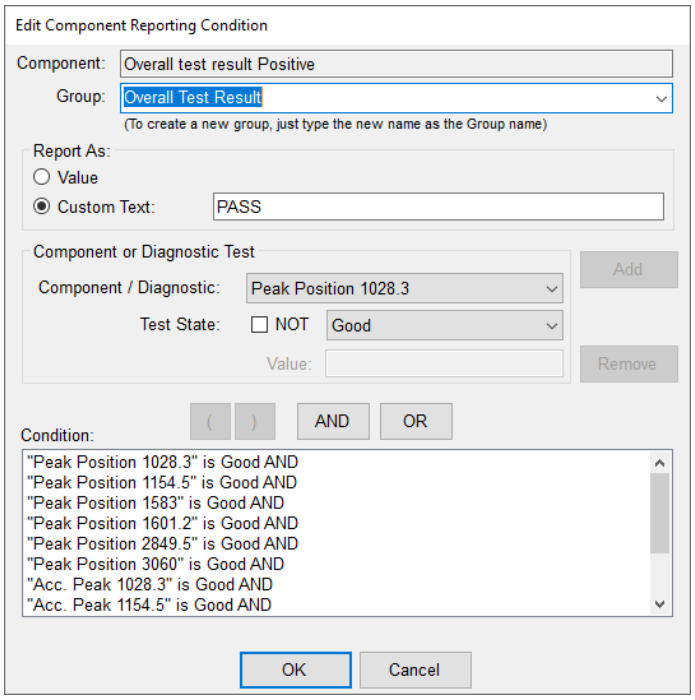

Figure 6. Conditions for overall positive test result

20 Select the component named “Overall test result Negative”.

21 Click **Edit**.

22 Change the **Group** to “Overall Test Result”.

23 Change **Report As** to “Custom” and add “FAIL”

24 Set the **Component / Diagnostic** to “[any_comp]”, tick the **NOT** checkbox, and click **Add.**

25 Click **OK**.

26 Use the Up and Down buttons to bring the components in the order seen in Figure 7:

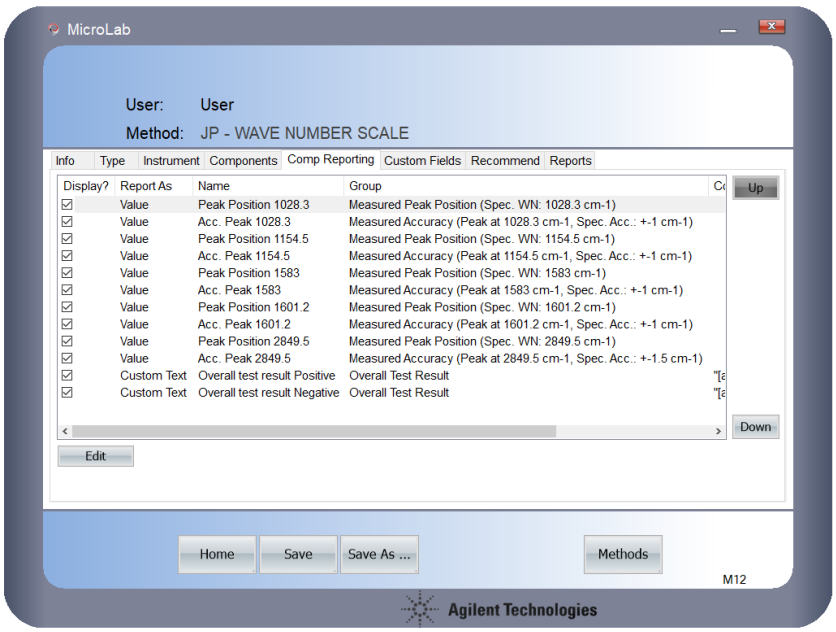

Figure 7. Components in correct order

27 Select the **Display?** check boxes for all components.

Setup the Outcome Positive test recommendation

1 Click the **Recommend** tab.

2 Click **Add**.

3 Change the Recommendation Name to “Test Outcome Positive”.

4 Set the **Component / Diagnostic** to “[all_comp]” and click **Add**.

5 Enter a descriptive **Recommendation** in the text box. We used “All test results are within acceptable limits. Details given below” for this example.

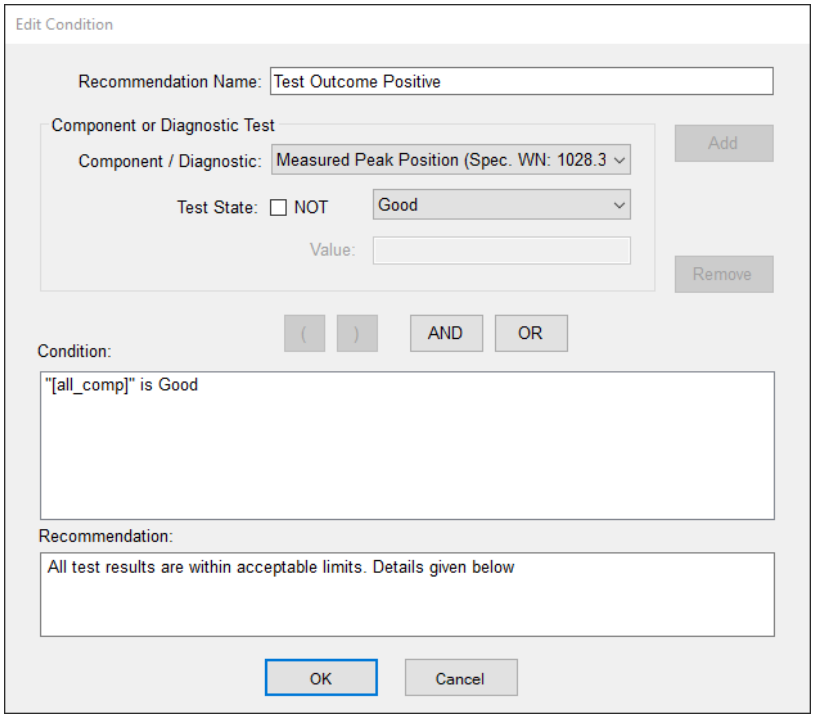

Figure 8. Example of test recommendation

6 Click **OK**.

Setup the Outcome Negative test recommendation and save the method

1 Click **Add**.

2 Change the Recommendation Name to “Test Outcome Negative”.

3 Set the **Component / Diagnostic** to “[any_comp]”, tick the **NOT** checkbox, and click **Add**.

4 Enter a descriptive **Recommendation** in the text box. We used “One or more of the test results are NOT within acceptable limits. Details given below” for this example.

5 Click **OK**.

6 Click **Save**.

3.2 Create a method for the Resolution Power

Create a copy of the “EP_TransRes_Poly_Test_Rev04” method

1 Click **Home**.

2 Click **Methods**.

3 Select the “EP_TransRes_Poly_Test_Rev04” method.

4 Click **Edit**.

5 Click **Save As… and** save the method with a descriptive file name. We used “JP – RESOLVING POWER”. for this example.

6 Click **Save**.

Setup the components tab

This procedure includes:

- Editing the test name and parameters for Resolution Test 1 and 2 (Steps 1-11)
- Editing parameters for outcomes of the Resolution Tests (Steps 12-15)

1 Select the created method and click **Edit** method.

2 Change the Y-Axis Units in Type to “**Transmittance**”.

3 Click the **Components** tab.

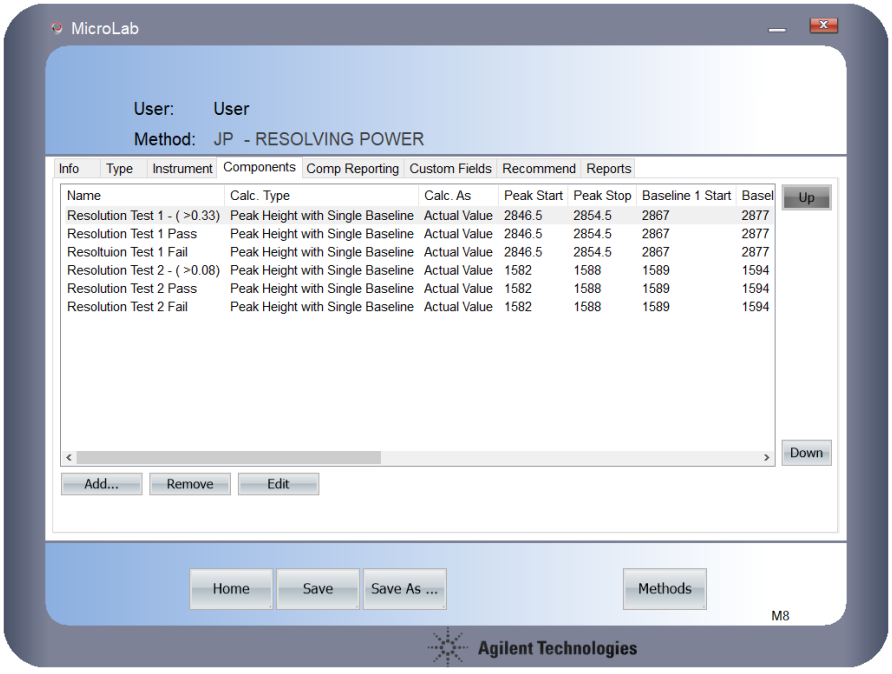

Figure 9. Initial Components tab with the “EP_TransRes_Poly_Test_Rev04” method imported

4 Select the component named “Resolution Test 1 – (>0.33)” and click **Edit**.

5 Change the Component Name to “Resolution Test 1 – (>=18)”.

6 Set up the component with the following parameters:

Component Name: "Resolution Test 1 – (>=18)".

Calculation: Select Peak Height with Single Baseline.

Peak Start: "2867".

Baseline 1Start: "2846.5"

Peak Stop: "2877".

Baseline 1Stop: "2854.5"

Decimal Digits To Report: "2".

Critical Low: "17.99".

7 Click OK.

8 Select the component named "Resolution Test 2 – (>0.08)" and click Edit.

9 Change the Component Name to "Resolution Test 2 – (>=12)".

10 Set up the component with the following parameters:

Component Name: "Resolution Test 2 – (>=12)".

Calculation: Select Peak Height with Single Baseline.

Peak Start: "1589".

Baseline 1 Start: "1582"

Peak Stop: "1594".

Baseline 1 Stop: "1588"

Decimal Digits To Report: "2".

Critical Low: "11.99".

11 Click OK.

12 Select the component named "Resolution Test 1 Pass" and click Edit.

13 Set up the component with the following parameters:

Component Name: "Resolution Test 1 Pass".

Calculation: Select Peak Height with Single Baseline.

Peak Start: "2867".

Baseline 1 Start: "2846.5"

Peak Stop: "2877".

Baseline 1 Stop: "2854.5"

Decimal Digits To Report: "2".

Critical Low: "17.99".

14 Click OK.

15 Repeat steps 12 to 14 with the details given in Table 6.

Table 6 Component parameters for various Resolution tests

Component Name	Calculation	Peak Start	Baseline 1 Start	Peak Stop	Baseline 1 Stop	Decimal Digits To Report	Offset (+Value)	Critical Low	Critical High
"Resolution Test 1 Fail"	Select Peak Height with Single Baseline	"2867"	"2846.5"	"2877"	"2854.5"	"2"	N/A	"17.99"	-
"Resolution Test 2 Pass"	Select Peak Height with Single Baseline	"1589"	"1582"	"1594"	"1588"	"2"	N/A	"11.99"	-
"Resolution Test 2 Fail"	Select Peak Height with Single Baseline	"1589"	"1582"	"1594"	"1588"	"2"	N/A	"11.99"	-
"Overall test result Positive"	Select Peak Height	"2867"	-	"2877"	-	"2"	"1000000"	"1"	-
"Overall test result Negative"	Select Peak Height	"2867"	-	"2877"	-	"2"	"1000000"	--	"1"

16 Use the Up and Down buttons to bring the components in the order seen in Figure 10.

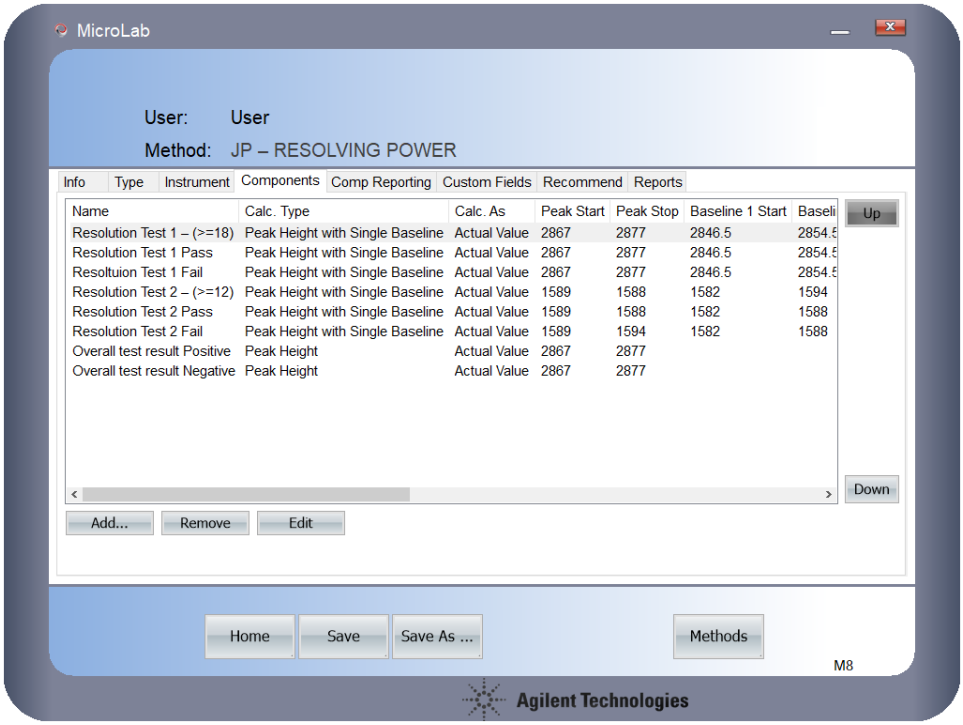

Figure 10. Components tab for the Resolving Power method

Setup the component reporting

This procedure includes:

- Creating the reporting method for Test 1 (Steps 2-17)
- Creating the reporting method for Test 2 (Steps 18-33)

1 Creating the reporting method for the Overall Test Results (Steps 34-49)Click the **Comp Reporting** tab.

2 Select the component named "Resolution Test 1 – (>=18)".

3 Click **Edit**.

4 Change the **Group** to “Test 1: The depth of the trough from the maximum absorption at about 2850 cm^{-1} to the minimum at about 2870 cm^{-1} (acceptance criterium >= 18%)”.
5 Click **OK**.
6 Select the component named “Resolution Test 1 Pass”.
7 Click **Edit**.
8 Change the **Group** to “Measured Accuracy (RESOLVING POWER – Test 1: Outcome)”.
9 Select the **Condition** and click **Remove.**
10 Set the **Component / Diagnostic** to “Resolution Test 1 – (>=18)” and click **Add.**
11 Click **OK**.
12 Select the component named “Resolution Test 1 Fail”.
13 Click **Edit**.
14 Change the **Group** to “Measured Accuracy (RESOLVING POWER – Test 1: Outcome)”.
15 Select the **Condition** and click **Remove.**
16 Set the **Component / Diagnostic** to “Resolution Test 1 – (>=18)” and tick the “NOT” check box and click **Add.**
17 Click **OK**.
18 Select the component named “Resolution Test 2 – (>=12)”.
19 Click **Edit**.
20 Change the **Group** to “Test 2: The depth of the trough from the maximum at about 1583 cm^{-1} to the minimum at about 1589 cm^{-1} (acceptance criterium >=12%)”.
21 Click **OK**.
22 Select the component named “Resolution Test 2 Pass”.
23 Click **Edit**.
24 Change the **Group** to “Measured Accuracy (RESOLVING POWER – Test 2: Outcome)”.
25 Select the **Condition** and click **Remove.**
26 Set the **Component / Diagnostic** to “Resolution Test 2 – (>=12)” and click **Add.**
27 Click **OK**.
28 Select the component named “Resolution Test 2 Fail”.
29 Click **Edit**.
30 Change the **Group** to “Measured Accuracy (RESOLVING POWER – Test 2: Outcome)”.
31 Select the **Condition** and click **Remove.**
32 Set the **Component / Diagnostic** to “Resolution Test 2 – (>=12)” and tick the “NOT” check box and click **Add.**
33 Click **OK**.
34 Select the component named “Overall test result Positive”.
35 Click **Edit**.
36 Change the **Group** to “Overall Test Result”.
37 Change **Report As** to “Custom” and add “PASS”.
38 Set the **Component / Diagnostic** to “Resolution Test 1 – (>=18)” and click **Add.**
39 Click **AND.**
40 Set the **Component / Diagnostic** to “Resolution Test 1 – (>=12)” and click **Add.**
41 Click **OK**.
42 Select the component named “Overall test result Negative”.

43 Click **Edit**.

44 Change the **Group** to “Overall Test Result”.

45 Change **Report As** to “Custom” and add “FAIL”.

46 Set the **Component / Diagnostic** to “Resolution Test 1 – (>=18)” and tick the “NOT” check box and click **Add.**

47 Click **OR.**

48 Set the **Component / Diagnostic** to “Resolution Test 1 – (>=12)” and tick the “NOT” check box and click **Add.**

49 Click **OK**.

50 Use the Up and Down buttons to bring the components in the order seen in Figure 11.

51 Select the **Display?** check boxes for all components.

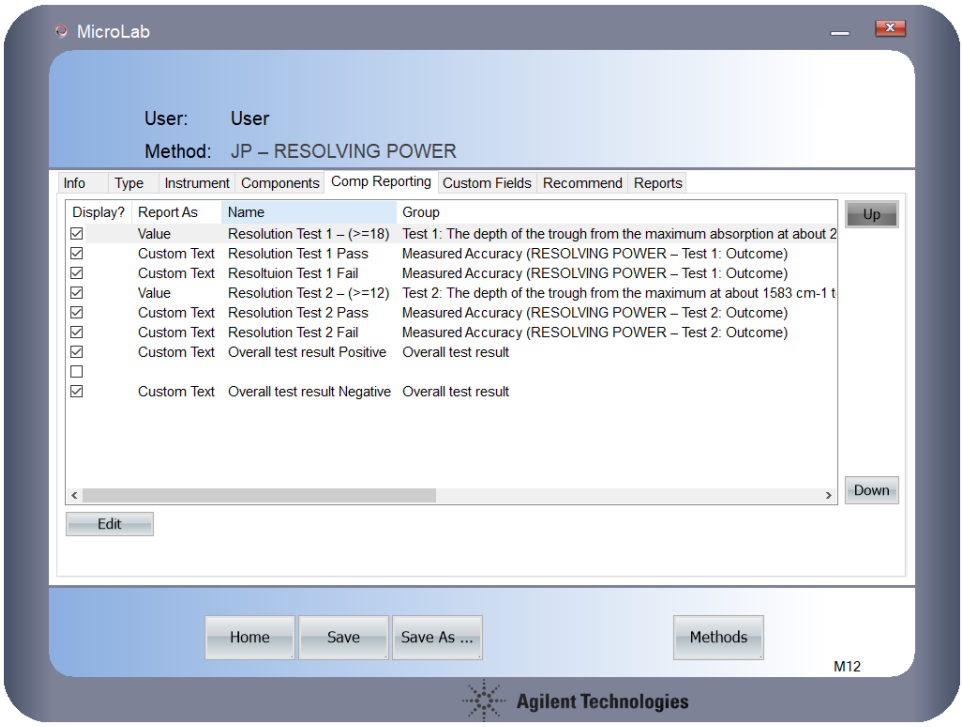

Figure 11. Comp Reporting tab for the Resolution Power method

Setup the test recommendation for the Positive Outcome

1 Click the **Recommend** tab.

2 Click **Add**.

3 Change the Recommendation Name to “Positive Outcome”.

4 Set the **Component / Diagnostic** to “[all_comp]” and click **Add**.

5 Enter a descriptive **Recommendation** in the text box. We used “All test results are within acceptable limits. Details given below” for this example.

6 Click **OK**.

Setup the test recommendation for the Negative Outcome and save the method

1 Click **Add**.

2 Change the Recommendation Name to “Negative Outcome”.

3 Set the **Component / Diagnostic** to "[any_comp]", tick the NOT checkbox, and click **Add**.

4 Enter a descriptive **Recommendation** in the text box. We used "One or more of the test results are NOT within acceptable limits. Details given below" for this example.

5 Click **OK**.

6 Click **Save**.

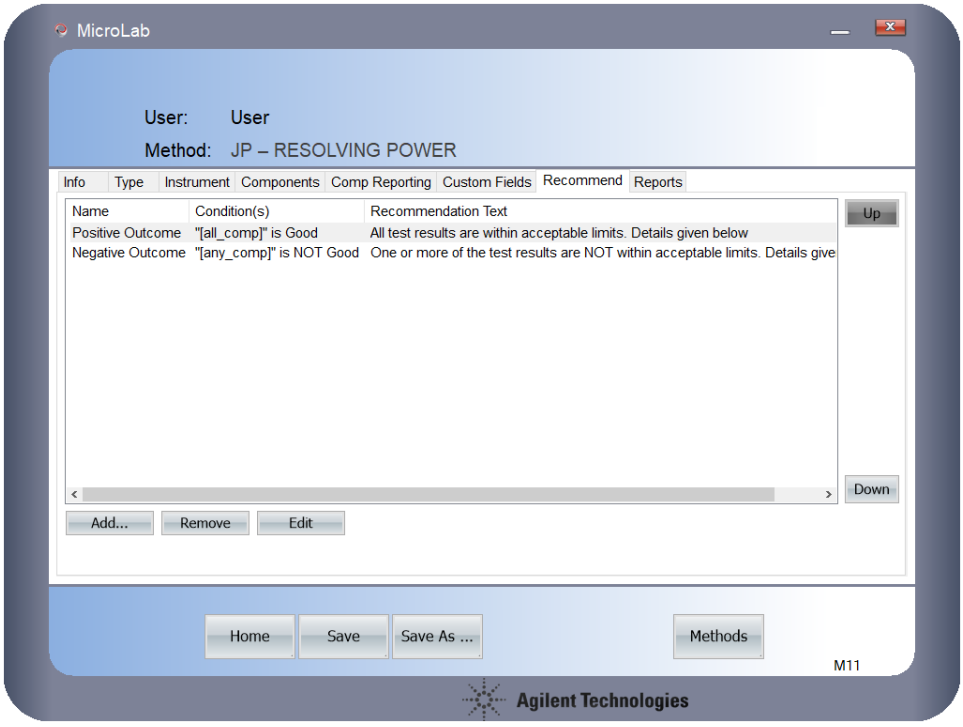

Figure 12. Recommend tab for the Resolution Power method

3.3 Create a method for the Wave Number Reproducibility and Transmittance Reproducibility

Create a new method

1 Click **New**.

2 Click **Save As... and** save the method with a descriptive file name. We used "JP – WAVE NUMBER REPRODUCIBILITY and TRANSMITTANCE REPRODDUCIBILITY" for this example.

3 Select the created method and click **Edit** method.

4 Click the **Type** tab.

5 Change the **Method** to "Components".

6 Change the **Y-Axis** to "Transmittance".

7 Click the **Instrument** tab.

8 Change the "Background Scans" to 140.

9 Change the "Sample scans" to 140.

10 Set the "Zero Fill Factor" to 8.

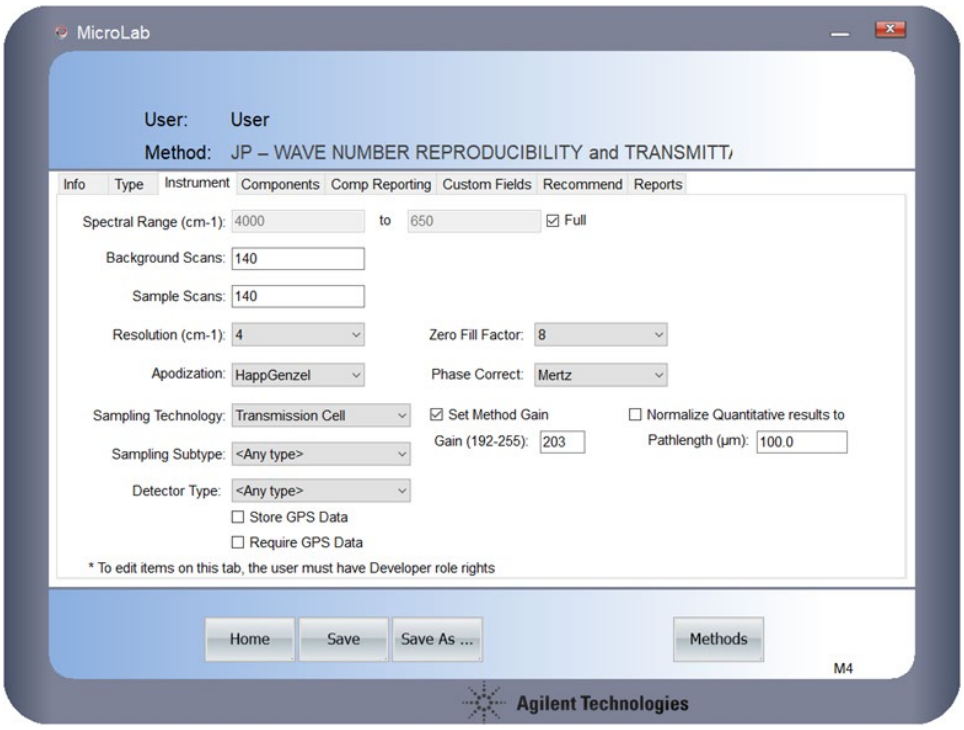

Figure 13. Instrument settings for the Wave Number Reproducibility and Transmittance Reproducibility method

Setup the components tab

1 Click the **Components** tab.

2 Click **Add.**

3 Set up the component with the following parameters:

Component Name: "Peak Position 3060"

Calculation: Select **Peak Position (Center of Gravity)**

Peak Start: "3060"

Peak Stop: "3060"

Decimal Digits To Report: "2"

4 Click **OK**.

5 Repeat steps 1 to 4 with the details given in Table 7.

Table 7 Component settings

Component Name	Calculation	Peak Start	Peak Stop	Decimal Digits To Report
"Peak Position 1028.3"	Peak Position (Center of Gravity)	1028.3	1028.3	2
"%T of band at ~3060 cm^{-1}"	Peak Height	3060	-	2
"%T of band at ~2849 cm^{-1}"	Peak Height	2849	-	2
"%T of band at ~1601 cm^{-1}"	Peak Height	1601	-	2
"%T of band at ~1583 cm^{-1}"	Peak Height	1583	-	2
"%T of band at ~1154.5 cm^{-1}"	Peak Height	1154.5	-	2
"%T of band at ~1028 cm^{-1}"	Peak Height	1028	-	2

Setup the component reporting

1 Click the **Comp Reporting** tab.

2 Select the component named “Peak Position 3060”.

3 Click **Edit**.

4 Change the **Group** to “WAVE NUMBER REPRODUCIBILITY: Wavenumber Position of band at about 3060 cm^{-1} ”.

5 Click **OK**.

6 Repeat steps 2 to 5 with the details given in Table 8.

Table 8 New group names

Component Name	New Group Name
“Peak Position 1028.3”	“WAVE NUMBER REPRODUCIBILITY: Wavenumber Position of band at about 1028 cm^{-1}”
“%T of band at ~3060 cm^{-1}”	“TRANSMITTANCE REPRODUCABILITY: %T of band at about 3060 cm^{-1}”
“%T of band at ~2849 cm^{-1}”	“TRANSMITTANCE REPRODUCABILITY: %T of band at about 2849 cm^{-1}”
“%T of band at ~1601 cm^{-1}”	“TRANSMITTANCE REPRODUCABILITY: %T of band at about 1601 cm^{-1}”
“%T of band at ~1583 cm^{-1}”	“TRANSMITTANCE REPRODUCABILITY: %T of band at about 1583 cm^{-1}”
“%T of band at ~1154 cm^{-1}”	“TRANSMITTANCE REPRODUCABILITY: %T of band at about 1154 cm^{-1}”
“%T of band at ~1028 cm^{-1}”	“TRANSMITTANCE REPRODUCABILITY: %T of band at about 1028 cm^{-1}”

7 Use the Up and Down buttons to bring the components in order seen in Figure 14:

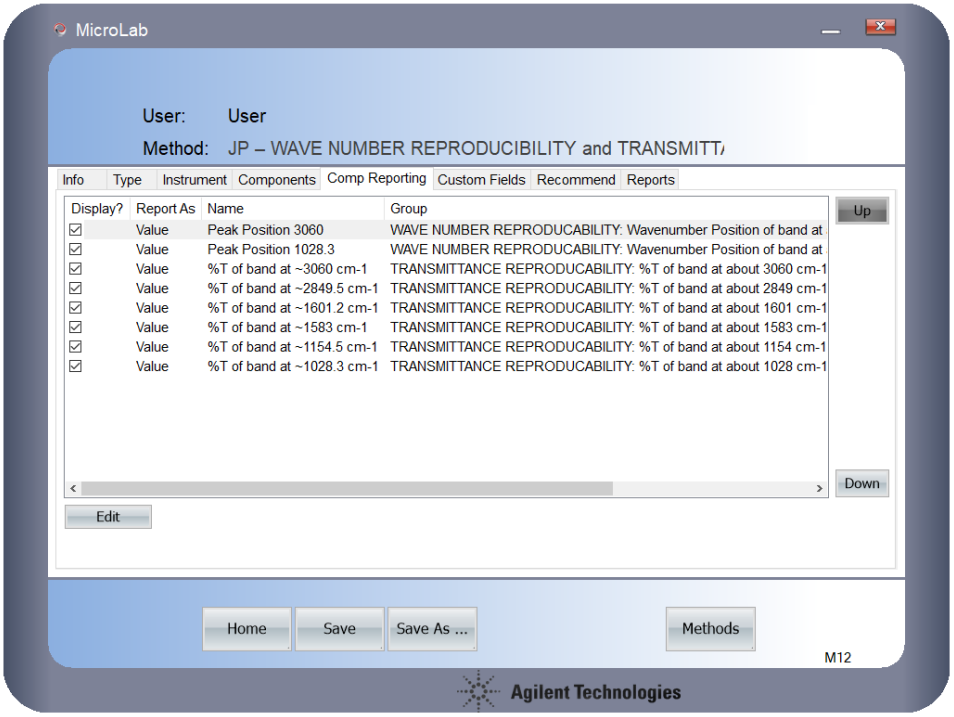

Figure 14. Comp reporting tab for the Wave Number Reproducibility and Transmittance method

8 Select the **Display?** check boxes for all components.

Setup the test recommendation and save the method

1. Click the Recommend tab.
2. Click Add.
3. Change the Recommendation Name to “rec0001”.
4. Set the Component / Diagnostic to [any comp]” and click Add.
5. Enter a descriptive Recommendation in the text box. We used “The WAVE NUMBER REPRODUCIBILITY and TRANSMISSION REPRODUCIBILITY test consists of two measurements. The results of these two measurements (Run 1 and Run 2) are used to manually calculate the relevant test results and compared against the limits.” for this example.
6. Click OK.
7. Click Save.

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4 Generating and Implementing Report Templates

The MicroLab software utilize customizable report templates to generate a pdf report of the measurement results.

There are several report templates that are supplied when the software is installed. They may be edited using Microsoft Word. However, it is highly recommended that the user save edited report templates as a different file name using the “Save As” function of word, so that the original templates are left intact.

When MicroLab PC is installed, it will also install an add-in to Microsoft Office’s Word platform. The add-in allows the user to customize or create report templates for use within the MicroLab software platform.

NOTE This feature is only supported on 32-bit installations of Microsoft Word 2010 or greater.

The use of this function requires knowledge of Microsoft Word that may not be covered in this manual.

4.1 Create/edit a report template

1. Open **Microsoft Word** and create a new document or edit a preinstalled report template.
2. Navigate to the **View menu/tab**.
3. A new feature has been added to the **View Menu** – **MicroLab Reporting**. This includes two buttons: **Report Designer** and **Perform Merge**.
4. To begin editing the document. Select the **Report Designer** function. The schema associated with MicroLab will appear as a menu on the right of the screen.

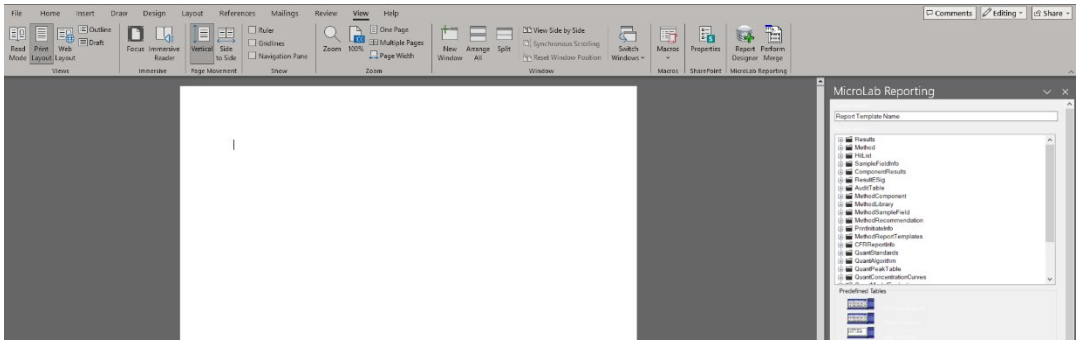

Figure 15. Microsoft Word with the MicroLab Reporting pane open

5. Give the Report Template a name in the **MicroLab Reporting Parameters** block (this name will later appear in the MicroLab software. Refer to Table 9 as an example.

Table 9 Example of MicroLab Reporting Parameters

Qualification Method Name	Report Template Name
JP – WAVE NUMBER SCALE	JP - WAVE NUMBER SCALE - Reporting.docx
JP – RESOLVING POWER	JP - RESOLVING POWER - Reporting.docx
JP – WAVE NUMBER REPRODUCIBILITY and TRANSMITTANCE REPRODDUCIBILITY	JP - WAVE NUMBER REPRODUCIBILITY and TRANSMITTANCE REPRODDUCIBILITY - Reporting.docx

4.2 Customize the report template

The Report Fields consist of parameter fields that are associated with the MicroLab Software. Fields can be located in a variety of categories for the user, from Results to Method Parameters.

1 To add fields to the report, simply click and drag the field desired to the report template page.

2 Add additional text, icons, etc. as required.

Examples of report templates for the three instrument qualification methods with the fields used and additional information given are shown below.

Report template examples

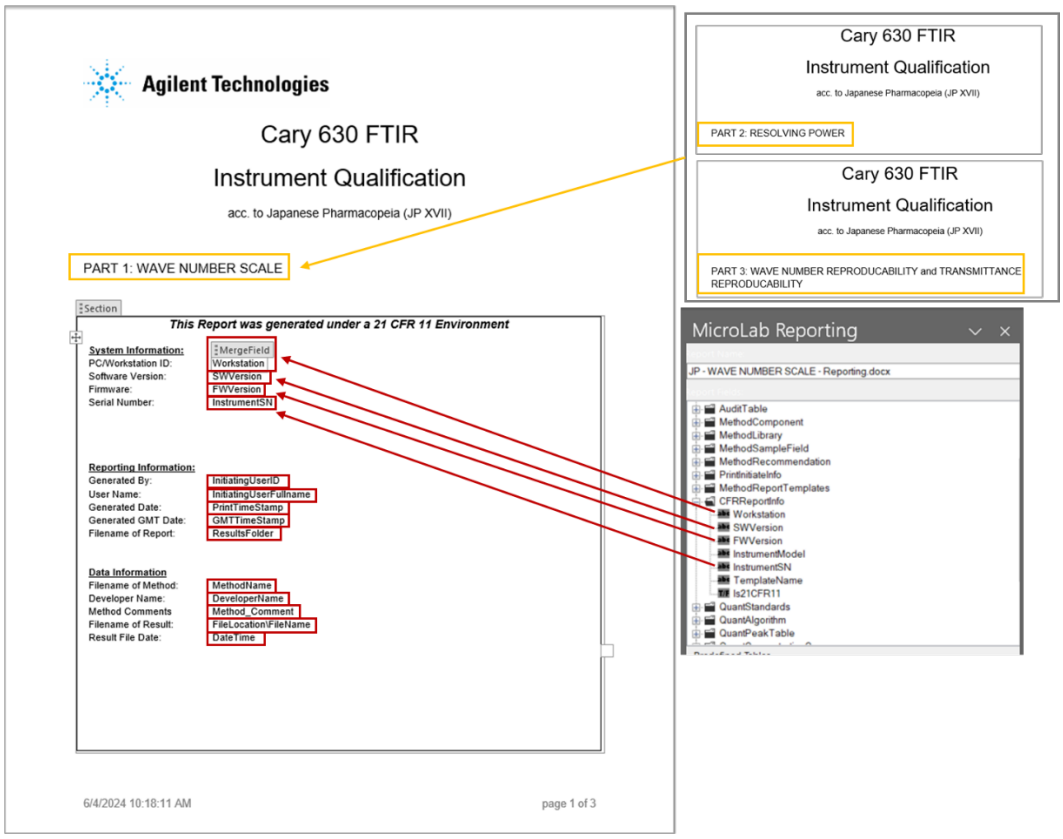

Figure 16. Title page example

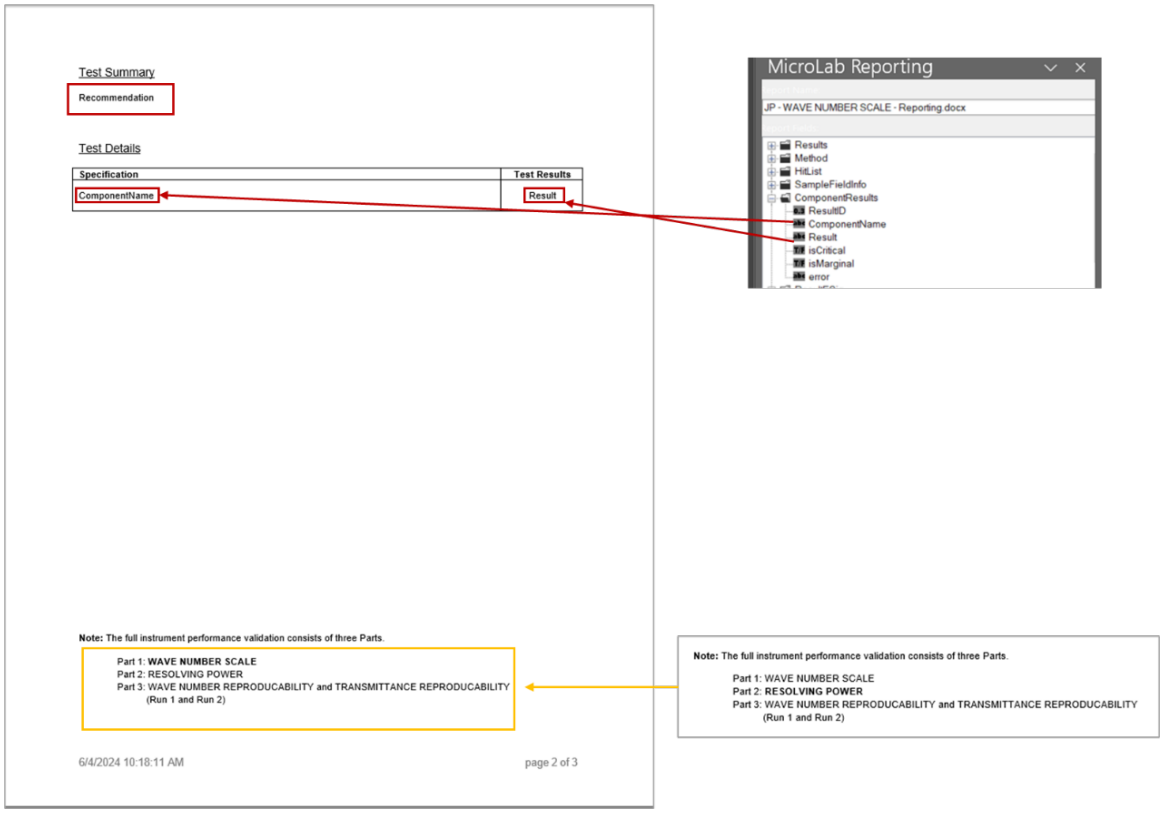

Figure 17. Example of "Test Summary" page for "JP – WAVE NUMBER SCALE" and "JP – RESOLVING POWER" methods

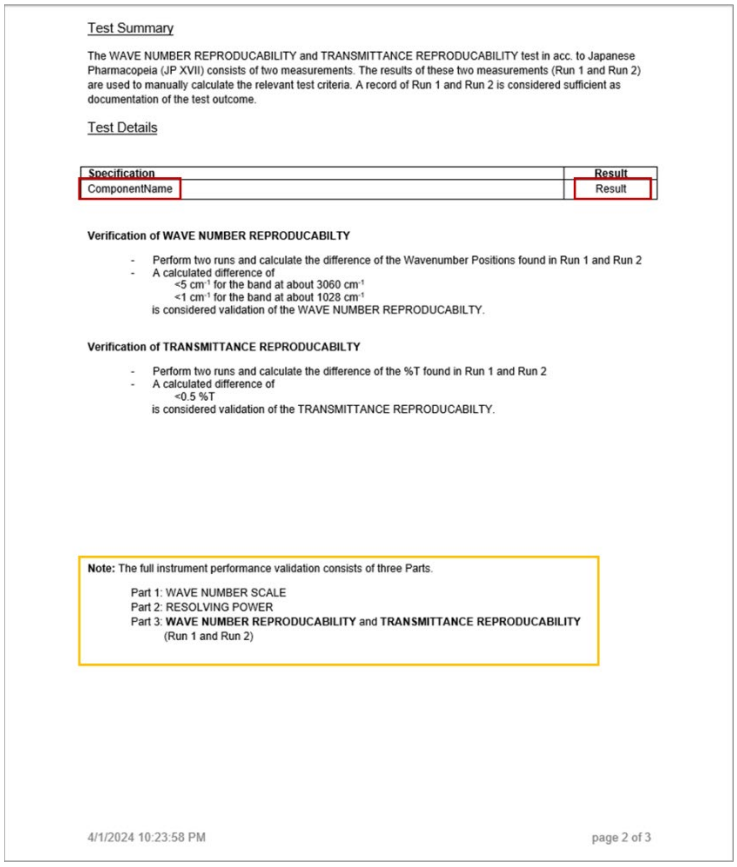

Figure 18. Example of "Title Test Summary" page for "JP – WAVE NUMBER REPRODUCIBILITY and TRANSMITTANCE REPRODDUCIBILITY" method

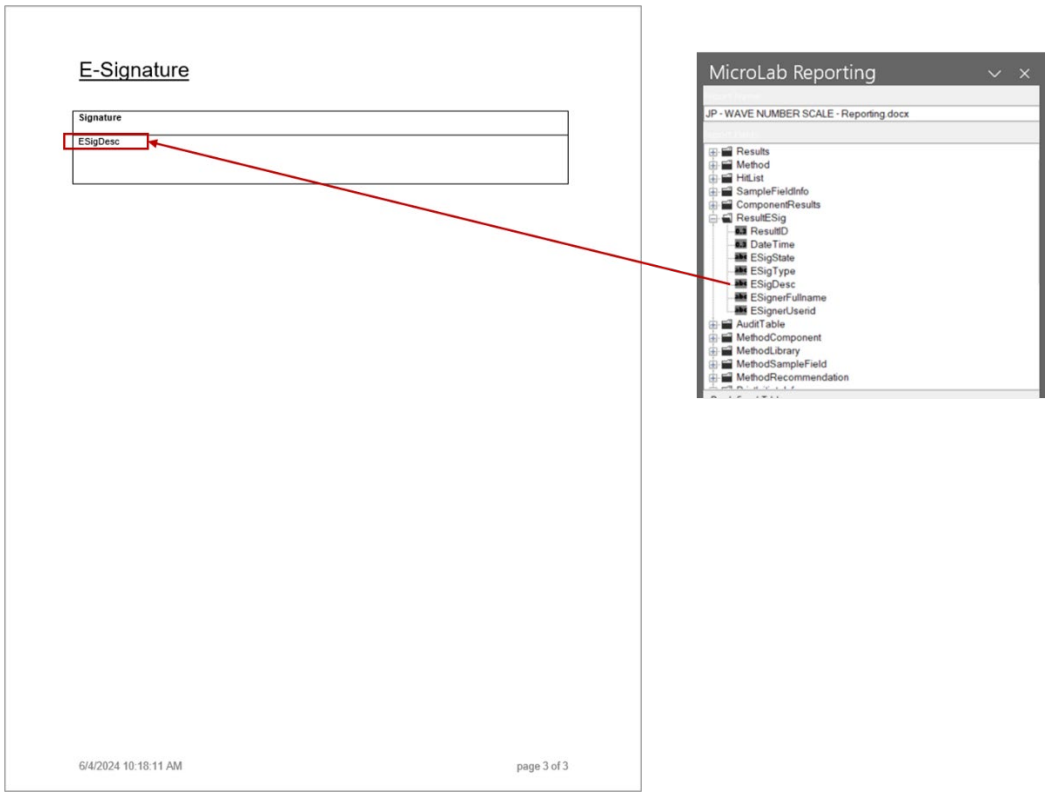

Figure 19. Example of an E-Signature page

Once the **Report** has been edited appropriately, the file should be saved to the report template folder for **MicroLab**. This folder is typically located in C:\Users\Public\Documents\Agilent\MicroLab\rptTemplates.

a

NOTE Save the file as docx file format.

4.3 Assign the report templates to the respective method

1. Open **MicroLab** or **MicroLab Lite**.
2. Select **Methods** from the **Home** screen and then select the method where a report template is desired. Select **Edit**.
3. From the method tabs, select **Reports**.
4. From the list of **Available Report Templates**, select the respective one to associate with the method. The naming convention that was suggested in Table 9 (see page 28) is shown in Figure 20.
5. Then click on the **Add** button.

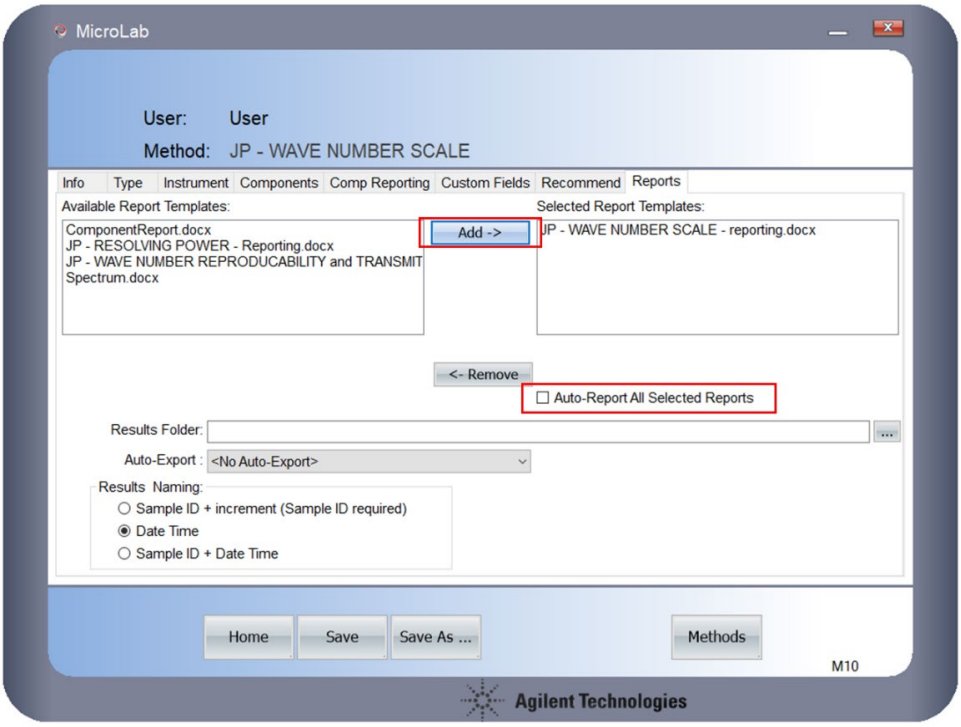

Figure 20. Reports tab

6 If automated report generation is desired, select the check box labeled **Auto-Report All Selected Reports**. This will automatically generate all associated reports at the end of the data analysis.

NOTE To remove an unwanted report, simply select the unwanted report and click the **Remove** button.

7 Once all changes have been made, click the **Save** button to save the method.

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5 Execution of the Instrument Qualification Methods

5.1 Preparing the Cary 630 FTIR

1. Connect the Cary 630 FTIR to the PC and switch it on.
2. Start MicroLab PC.
3. Attach the Transmission module to the Cary 630 FTIR engine.

5.2 Performing the Wave Number Scale test

1. Click Methods.
2. Select the "JP – WAVE NUMBER SCALE" method.
3. Click Activate.
4. Click Start on the Home screen.
5. When prompted, ensure that no sample is present in the sample compartment.
6. Click Next. A "crystal check" and "background collect" are performed.

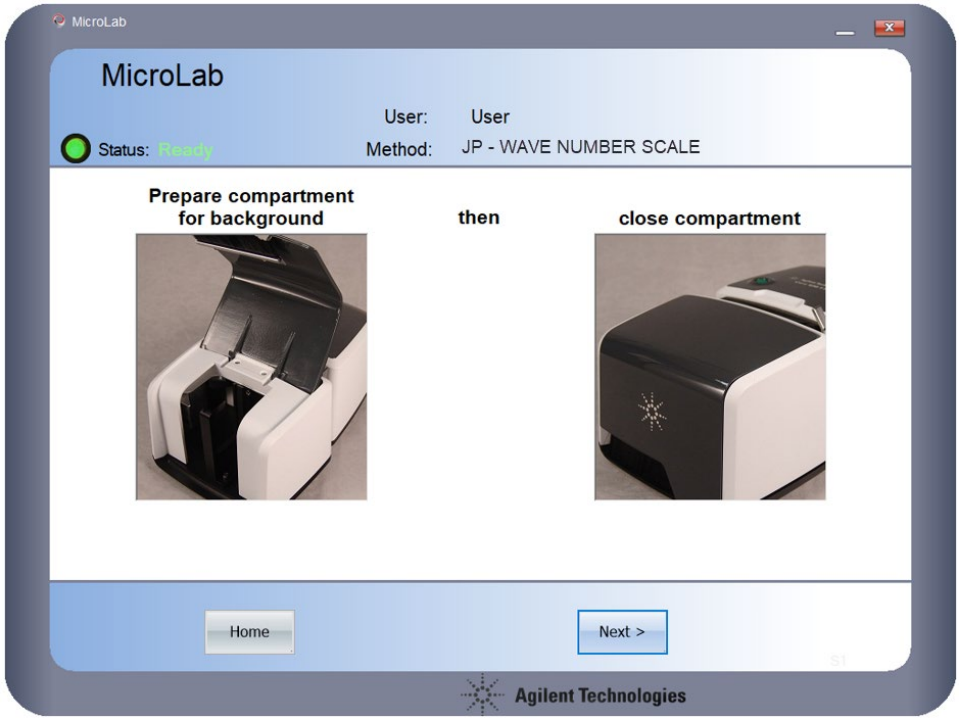

Figure 21. Method start screen

7 Place the traceable polystyrene film card into the sample holder in the instrument sample compartment and click **Next**.

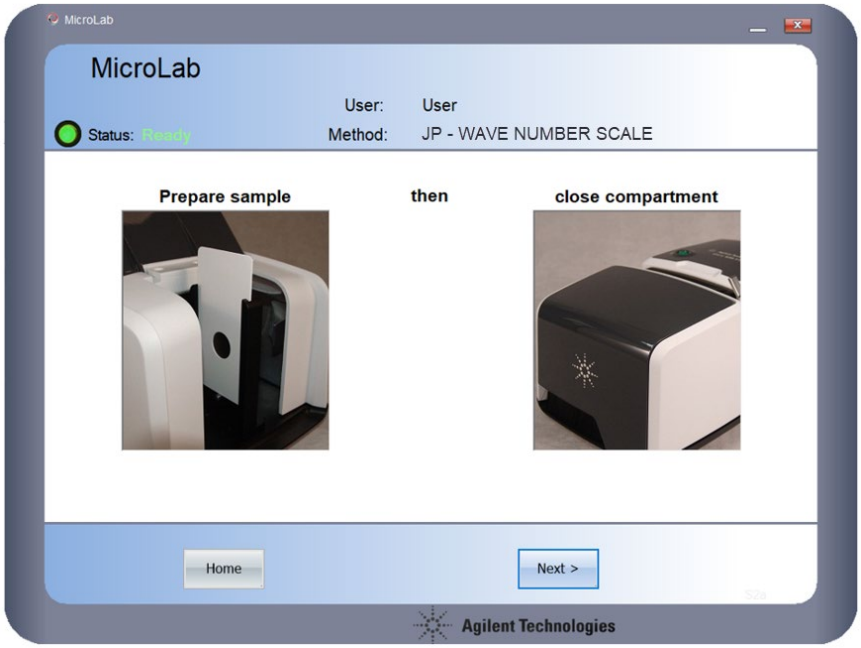

Figure 22. Sample preparation prompt screen

8 When prompted, enter a descriptive Sample ID.

9 Click **Next**. A sample measurement will be performed.

10 Review the results.

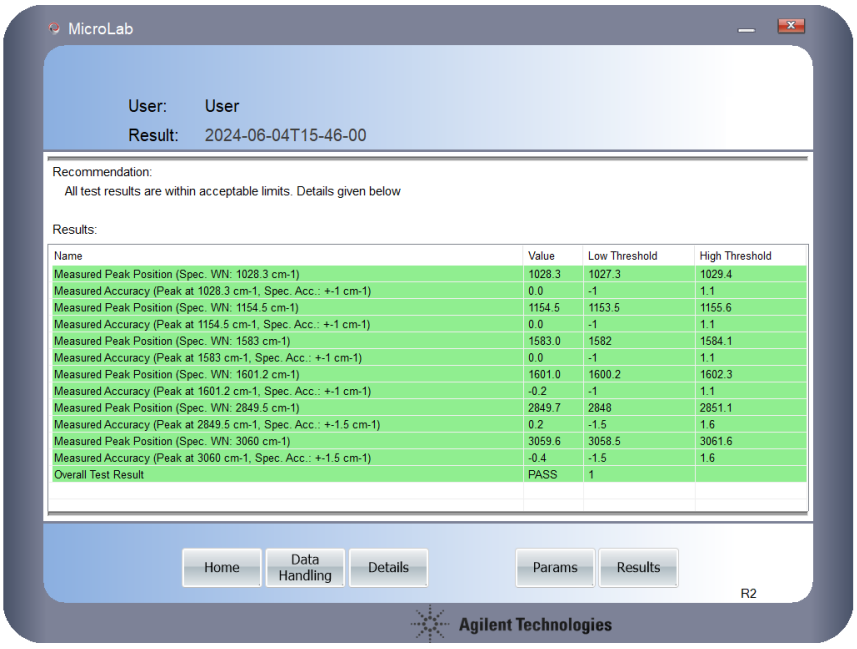

Figure 23. An example of the results from a Wave Number Scale test

11 Click **Done**.

5.3 Performing the Resolution Power test

1 Click **Methods**.
2 Select the “JP – RESOLVING POWER” method.
3 Click **Activate**.
4 Click **Start** on the **Home** screen.
5 When prompted, ensure that no sample is present in the sample compartment.
6 Click **Next**. A “crystal check” and “background collect” are performed.

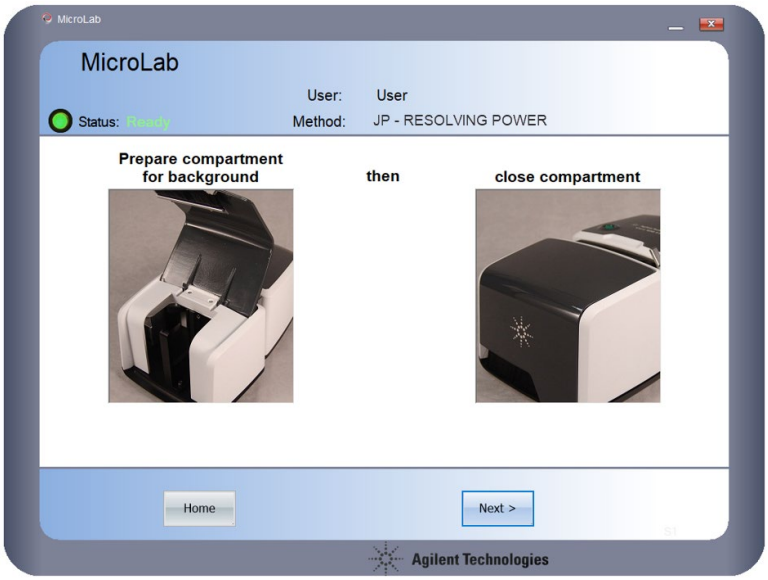

Figure 24. Method start screen

7 Place the traceable polystyrene film card into the sample holder in the instrument sample compartment and click **Next**.

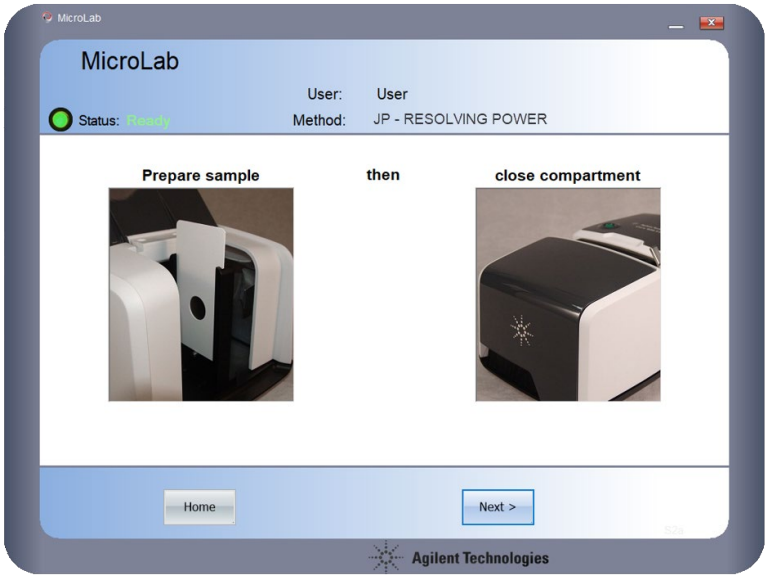

Figure 25. Sample preparation prompt screen

8 When prompted, enter a descriptive Sample ID.

9 Click **Next**. A sample measurement will be performed.

10 Review the results.

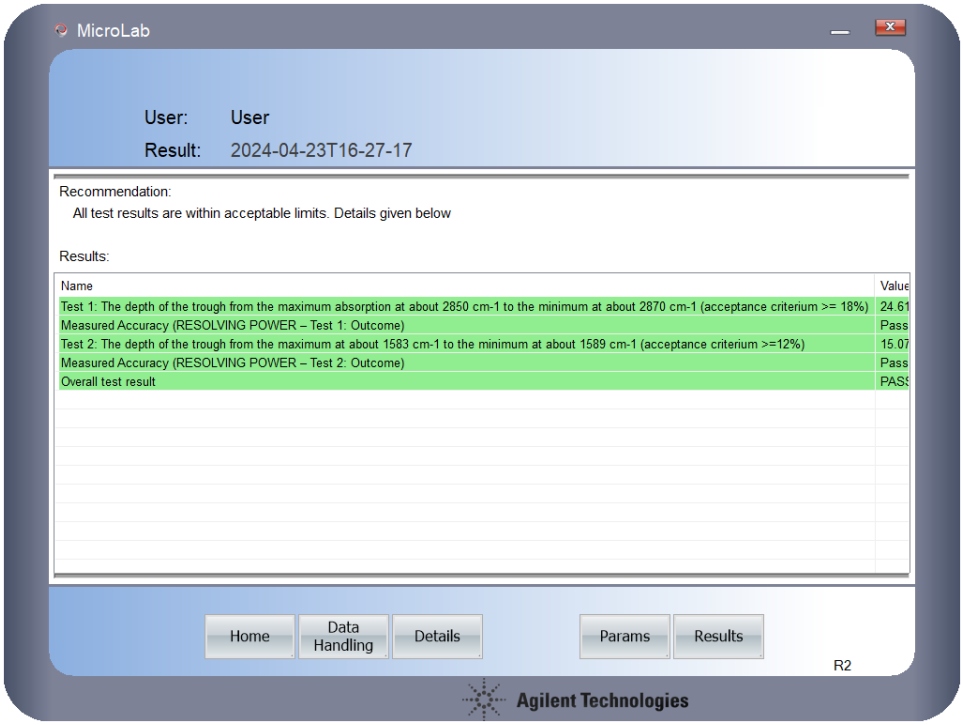

Figure 26. An example of the results from a Resolution Power test

11 Click **Done**.

5.4 Perform the Wave Number Reproducibility and Transmittance Reproducibility test

This test requires the operator to perform two measurements and then to compare the individual results of these measurements.

1 Click **Methods**.

2 Select the “JP – WAVE NUMBER REPRODUCIBILITY and TRANSMITTANCE REPRODDUCIBILITY” method.

3 Click **Activate**.

4 Click **Start** on the **Home** screen.

5 When prompted, ensure that no sample is present in the sample compartment.

6 Click **Next**. A “crystal check” and “background collect” are performed.

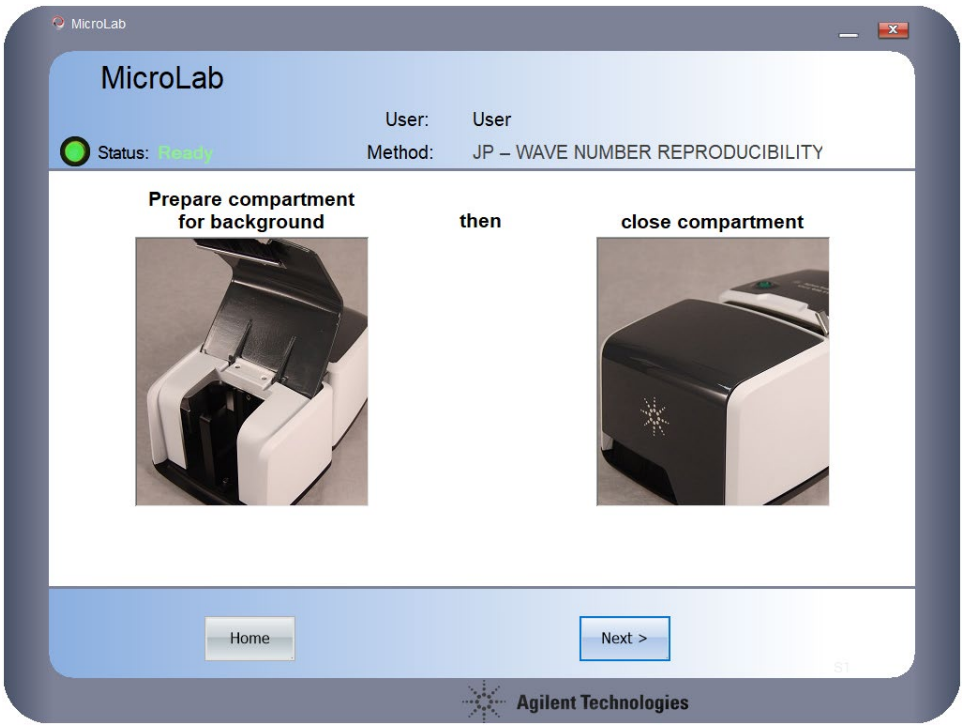

Figure 27. Method start screen.

7 Place the traceable polystyrene film card into the sample holder in the instrument sample compartment and click **Next**.

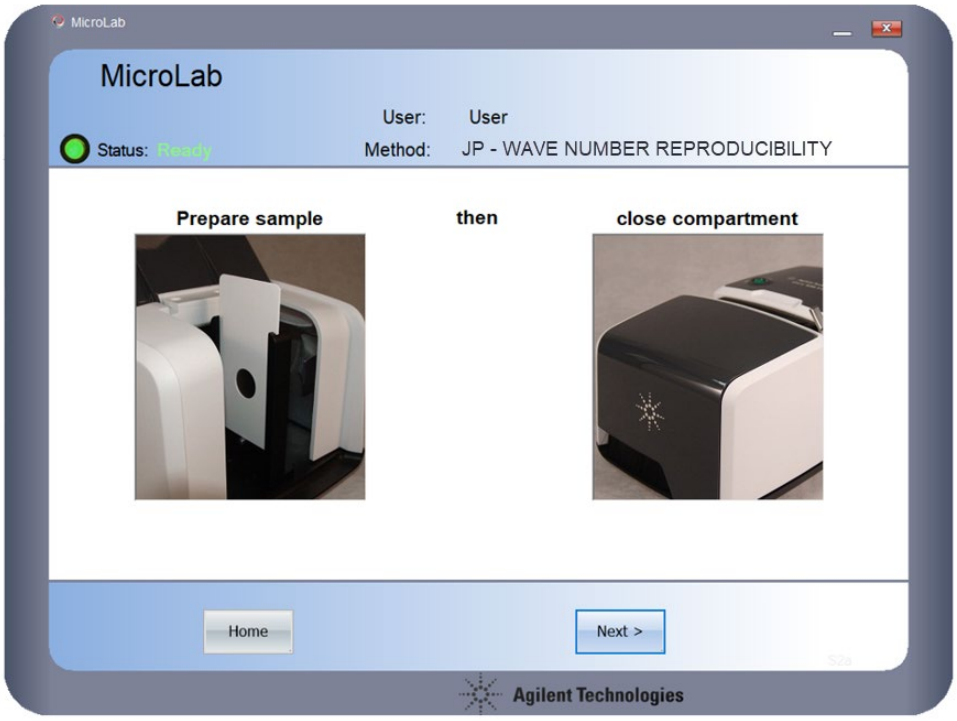

Figure 28. Sample preparation prompt screen

8 When prompted, enter a descriptive Sample ID.

9 Click **Next**. A sample measurement will be performed.

10 Review the results.

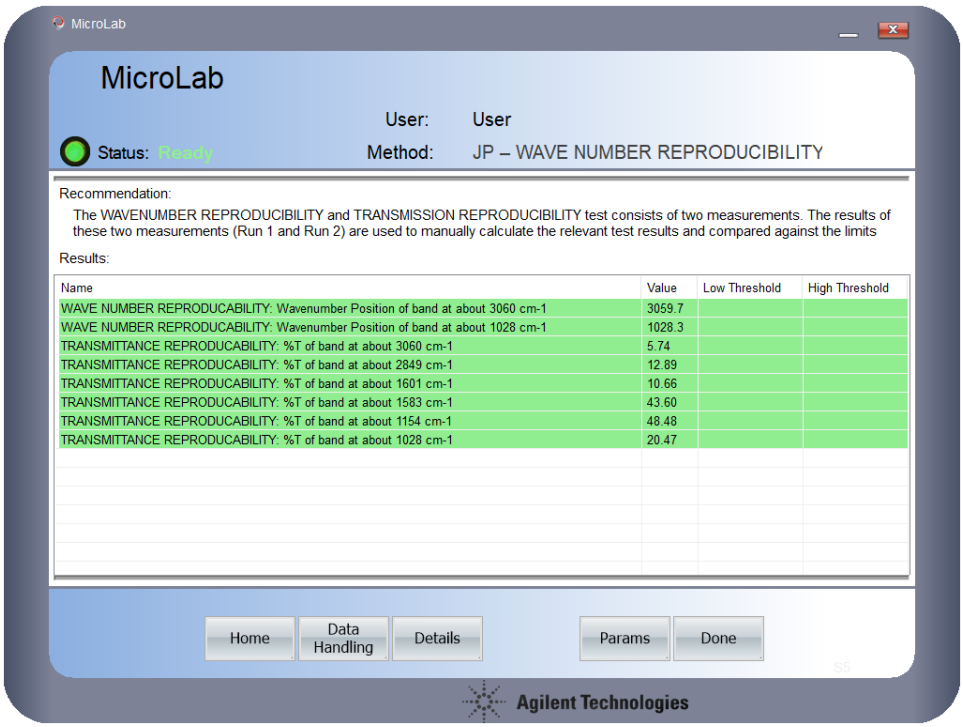

Figure 29. An example of the results from a Wave Number Reproducibility test

11 Click **Done**.

12 Repeat steps 5 to 9. At step 8 add a comment: Reference to sample ID of first measurement and record result, e.g.:

"Result from 1st measurement (sample) ID:

Wave Number Reproducibility:

Wavenumber Position of band at about 1028 cm^{-1}:

Wavenumber Position of band at about 3060 cm^{-1}:

TRANSMITTANCE REPRODUCIBILITY:

%T of band at about 3060 cm^{-1}:

%T of band at about 2849 cm^{-1}:

%T of band at about 1601 cm^{-1}:

%T of band at about 1583 cm^{-1}:

%T of band at about 1154 cm^{-1}:

%T of band at about 1028 cm^{-1}:"

13 Review the results and manually calculate the differences for the results between the two measurements and compare the calculated differences to the test limits given in Table 10:

Table 10 Manual pass or fail checker

	Result from measurement 1	Result from measurement 2	Difference between results from measurement 1 from measurement 2	Test limit	Pass/Fail
Wave Number reproducibility					
Wavenumber Position of band at about 3060 cm^{-1}				<5 cm^{-1}	
Wavenumber Position of band at about 1028 cm^{-1}				<1 cm^{-1}	
TRANSMITTANCE REPRODUCIBILITY					
%T of band at about 3060 cm^{-1}				<0.5%	
%T of band at about 2849 cm^{-1}					
%T of band at about 1601 cm^{-1}					
%T of band at about 1583 cm^{-1}					
%T of band at about 1154 cm^{-1}					
%T of band at about 1028 cm^{-1}					

If all calculated differences are within the limits the test is considered a “pass”.

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In This Document

The manual describes the following:

- Scope
- Equipment and Materials
- Method Development
- Generating and Implementing Report Templates
- Execution of the Instrument Qualification Methods

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