

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

**Instruction Sheet** 



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## Scope

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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.

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

Table 1	JP system verification	test descriptions and	test limits
---------	------------------------	-----------------------	-------------

(1) The band at around 1942.9 cm<sup>-1</sup> 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.

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#### 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

2.1 Materials2.2 Instrumentation

7 7

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  $\mu$ m 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

**Equipment and Materials** 

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## 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.

Microl	Lab	- 🔳
	User: User Method: Default	
	method: Deradit	
	Methods	Edit/Create Methods
	Reference Methods	Reference Method Info
	Exit	Exits the application
		Draviaue Deculte Advanced Features
		Previous Results Advanced Features L1

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.

	Use	er: U	ser				
O Status: Reedy	Metho	od: Jl	- WAV	ENUMBER S	CALE		
Info Type Instrument Components	Comp Report	ing Custon	n Fields Re	commend Repo	orts		
Name Calc. Type	Calc. As	Peak Start	Peak Stop	Baseline 1 Start	Baseline 1 Stop	Baseline	Up
Peak1 Peak Position (Center of Gravity)	Actual Value	906.6	906.6				
Peak2 Peak Position (Center of Gravity)	Actual Value	1028.3	1028.3				
Peak3 Peak Position (Center of Gravity)	Actual Value	1154.5	1154.5				
Peak4 Peak Position (Center of Gravity)	Actual Value	1583	1583				
Peak5 Peak Position (Center of Gravity)	Actual Value	1601.2	1601.2				
Peak6 Peak Position (Center of Gravity)	Actual Value	2849.5	2849.5				
							Down
Add Remove Edit						7	

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".

Edit Component	$\times$
Component Name: Peak Position 1028.3	
Calculation Calculation Type: Peak Position (Center of Gravity) ~	
Peak Start: 1028.3 Peak Stop: 1028.3	
Baseline 1 Start: Baseline 1 Stop:	
Baseline 2 Start: Baseline 2 Stop:	
Scaling       Invert (1/Value)       Decimal Digits To Report:       1       Scale (x Value):       Offset (+ Value):	
Thresholds       Marginal Low:       Marginal High:         Critical Low:       1027.3       Critical High:       1029.4	
Calc Value As: Actual Value  V To Select a Percent type, you must enter  at least a Critical High value.	
OK Cancel	

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.

Old component	New component name	Decimal Digits	Thresholds	
name		To Report	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

Table 2 Component parameters for Peak3 to Peak7

#### 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.

	ι	lser: l	Jser							
	Ν	/lethod:	JP - WAVE	NUMBER SC	ALE					
Info	Туре	Instrument	Components	Comp Reporting	Custom Fields	Recommer	d Reports			
Nam	ne		Calc. Type		Calc. As	Peak Start	Peak Stop	Baseline 1 Start	Baseli	Up
Pea	k Positior	n 1028.3	Peak Position	(Center of Gravit	y) Actual Value	1028.3	1028.3			
Acc	Peak 10	28.3	Peak Position	(Center of Gravit	y) Actual Value	1028.3	1028.3			
Pea	k Positior	n 1154.5	Peak Position	(Center of Gravit	y) Actual Value	1154.5	1154.5			
Acc.	. Peak 11	54.5	Peak Position	(Center of Gravit	y) Actual Value	1154.5	1154.5			
Pea	k Positior	1583	Peak Position	(Center of Gravit	y) Actual Value	1583	1583			
Acc.	Peak 15	83	Peak Position	(Center of Gravit	y) Actual Value	1583	1583			
Pea	k Positior	1601.2	Peak Position	(Center of Gravit	y) Actual Value	1601.2	1601.2			
Acc.	Peak 16	01.2	Peak Position	(Center of Gravit	y) Actual Value	1601.2	1601.2			
Pea	k Positior	1 2849.5	Peak Position	(Center of Gravit	y) Actual Value	2849.5	2849.5			
Acc.	Peak 28	49.5	Peak Position	(Center of Gravit	y) Actual Value	2849.5	2849.5			
Ove	rall test r	esuit Positive	Peak Position	(Center of Gravit	y) Actual value	1583	1583			
Ove	rall test r	esult ivegative	Peak Position	(Center of Gravit	y) Actual value	1583	1583			
										Down
				_						
A	\dd	Remove	Edit							

Figure 4. Components tab

#### Setup the component reporting

- 1 Click the Comp Reporting tab.
- 2 Select the component named "Peak Position 1028.3".

Name Peak Position 1028.3 Peak Position 1154.5 Peak Position 1583 Peak Position 1601.2 Peak Position 2849.5 Peak Position 3060	Group Peak2 Peak3 Peak4 Peak5 Peak6	C	iondition(s) Custom T	ext	Up
Peak Position 1028.3 Peak Position 1154.5 Peak Position 1583 Peak Position 1601.2 Peak Position 2849.5 Peak Position 3060	Peak2 Peak3 Peak4 Peak5 Peak6				
Peak Position 1154.5 Peak Position 1583 Peak Position 1601.2 Peak Position 2849.5 Peak Position 3060	Peak3 Peak4 Peak5 Peak6				
Peak Position 1583 Peak Position 1601.2 Peak Position 2849.5 Peak Position 3060	Peak4 Peak5 Peak6				
Peak Position 1601.2 Peak Position 2849.5 Peak Position 3060	Peak5 Peak6				
Peak Position 2849.5 Peak Position 3060	Peak6				
Peak Position 3060					
	Peak7				
Acc. Peak 1028.3	Acc. Peak 1028.	3			
Acc. Peak 1154.5	Acc. Peak 1154.	5			
Acc. Peak 1583	Acc. Peak 1583				
Acc. Peak 1601.2	1601.2				
Acc. Peak 2849.5	Acc. Peak 2849.	5			
Acc. Peak 3060	Acc. Peak 3060				
Overall test result Positive	Overall test resul	t Positive			
Overall test result Negative	e Overall test resul	t Negative			Down
	Acc. Peak 1583 Acc. Peak 1601.2 Acc. Peak 2849.5 Acc. Peak 3060 Overall test result Positive Overall test result Negative	Acc. Peak 1583         Acc. Peak 1583           Acc. Peak 1601.2         1601.2           Acc. Peak 2849.5         Acc. Peak 2849.5           Acc. Peak 3060         Acc. Peak 3060           Overall test result Positive         Overall test result	Acc. Peak 1583         Acc. Peak 1583           Acc. Peak 1601.2         1601.2           Acc. Peak 2849.5         Acc. Peak 2849.5           Acc. Peak 3060         Acc. Peak 3060           Overall test result Positive         Overall test result Positive           Overall test result Negative         Overall test result Negative	Acc. Peak 1583         Acc. Peak 1583           Acc. Peak 1601.2         1601.2           Acc. Peak 2849.5         Acc. Peak 2849.5           Acc. Peak 3060         Acc. Peak 3060           Overall test result Positive         Overall test result Positive           Overall test result Negative         Overall test result Negative	Acc. Peak 1583         Acc. Peak 1583           Acc. Peak 1601.2         1601.2           Acc. Peak 2849.5         Acc. Peak 2849.5           Acc. Peak 3060         Acc. Peak 3060           Overall test result Positive         Overall test result Positive           Overall test result Negative         Overall test result Negative

Figure 5. Component "Acc. Peak 1028.3" selected

- 3 Click Edit.
- 4 Change the Group to "Measured Peak Position (Spec. WN: 1028.3 cm<sup>-1</sup>)".
- 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 <sup>-1</sup> )"
"Peak Position 1583"	"Measured Peak Position (Spec. WN: 1583 cm <sup>-1</sup> )"
"Peak Position 1601.2"	"Measured Peak Position (Spec. WN: 1601.2 cm <sup>-1</sup> )"
"Peak Position 2849.5"	"Measured Peak Position (Spec. WN: 2849.5 cm <sup>-1</sup> )"
"Peak Position 3060"	"Measured Peak Position (Spec. WN: 3060 cm <sup>-1</sup> )"

- 7 Select the component named "Acc. Peak 1028.3".
- 8 Click Edit.
- 9 Change the Group to "Measured Accuracy (Peak at 1028.3 cm<sup>-1</sup>, Spec. Acc.: +-1 cm<sup>-1</sup>)".
- 10 Click OK.
- **11** Repeat steps 7 to 10 with the details given in Table 5.

Table 5	New group names for Acc. Peaks
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Component Name	New Group Name
"Acc. Peak 1154.5"	"Measured Accuracy (Peak at 1154.5 cm <sup>-1</sup> , Spec. Acc.: +-1 cm <sup>-1</sup> )"
"Acc. Peak 1583"	"Measured Accuracy (Peak at 1583 cm <sup>-1</sup> , Spec. Acc.: +-1 cm <sup>-1</sup> )"
"Acc. Peak 1601.2"	"Measured Accuracy (Peak at 1601.2 cm <sup>-1</sup> , Spec. Acc.: +-1 cm <sup>-1</sup> )"
"Acc. Peak 2849.5"	"Measured Accuracy (Peak at 2849.5 cm <sup>-1</sup> , Spec. Acc.: +-1.5 cm <sup>-1</sup> )"
"Acc. Peak 3060"	"Measured Accuracy (Peak at 3060 cm <sup>-1</sup> , Spec. Acc.: +-1.5 cm <sup>-1</sup> )"

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.

Edit Component Reporting Condition
Component: Overall test result Positive
Group: Overall Test Result.
(To create a new group, just type the new name as the Group name) Report As: O Value O Custom Text: PASS
Component or Diagnostic Test
Component / Diagnostic: Peak Position 1028.3
Test State: NOT Good ~
Value: Remove
Condition:
"Peak Position 1028.3" is Good AND         "Peak Position 1154.5" is Good AND         "Peak Position 1583" is Good AND         "Peak Position 1601.2" is Good AND         "Peak Position 2849.5" is Good AND         "Peak Position 3060" is Good AND         "Peak Position 3060" is Good AND         "Acc. Peak 1028.3" is Good AND         "Acc. Peak 1154.5" is Good AND         "Acc. Peak 1154.5" is Good AND
OK Cancel

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:

Di	DesertAs	Mana	0	
Display	Kepon As	Name	Group	Up Up
	Value	Acc. Posk 1029.2	Measured Accuracy (Reak at 1029.2 cm 1, Spec. Acc.: + 1 cm 1)	
	Value	Peak Position 1154 5	Measured Peak Position (Spec. W/N: 1154.5 cm.1)	
2	Value	Acc. Peak 1154.5	Measured Accuracy (Peak at 1154.5 cm-1, Spec, Acc.: +-1 cm-1)	
	Value	Peak Position 1583	Measured Peak Position (Spec. WN: 1583 cm-1)	
M	Value	Acc. Peak 1583	Measured Accuracy (Peak at 1583 cm-1, Spec, Acc.: +-1 cm-1)	
2	Value	Peak Position 1601.2	Measured Peak Position (Spec. WN: 1601.2 cm-1)	
	Value	Acc. Peak 1601.2	Measured Accuracy (Peak at 1601.2 cm-1, Spec. Acc.: +-1 cm-1)	
	Value	Peak Position 2849.5	Measured Peak Position (Spec. WN: 2849.5 cm-1)	
	Value	Acc. Peak 2849.5	Measured Accuracy (Peak at 2849.5 cm-1, Spec. Acc.: +-1.5 cm-1)	
	Custom Text	Overall test result Positive	Overall Test Result	"[a
	Custom Text	Overall test result Negative	Overall Test Result	"[2
<				> Down
Edit				

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.

Edit Condition	
Recommendation Name: Test Outcome Positive	
Component or Diagnostic Test	
Component / Diagnostic: Measured Peak Position (Spec. WN: 1028.3 $\sim$	Add
Test State: 🗌 NOT 🛛 Good 🗸 🗸	
Value:	Remove
Condition:	
"[all_comp]" is Good	
Recommendation:	
All test results are within acceptable limits. Details given below	
OK Cancel	

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.

		strument	Components	Comp Repo	orting C	ustom Fields	Recommen	d Reports			
ame			Calc. Type			Calc. As	Peak Start	Peak Stop	Baseline 1 Start	Basel	Up
esolution	Test 1	- ( >0.33)	Peak Height	with Single E	Baseline	Actual Value	2846.5	2854.5	2867	2877	
esolution	Test 1	Pass	Peak Height	with Single E	Baseline	Actual Value	2846.5	2854.5	2867	2877	
esoltuion	Test 1	Fail	Peak Height	with Single E	Baseline	Actual Value	2846.5	2854.5	2867	2877	
esolution	Test 2	- ( >0.08)	Peak Height	with Single E	aseline	Actual Value	1582	1588	1589	1594	
esolution	Test 2	Pass	Peak Height	with Single E	Baseline	Actual Value	1582	1588	1589	1594	
										>	Down
Add		Remove	Edit								
	Anne esolution esolution esolution esolution esolution	Add	Add	Imme     Calc. Type       essolution Test 1 - (>0.33)     Peak Height 1       essolution Test 1 Pass     Peak Height 1       essolution Test 1 Fail     Peak Height 1       essolution Test 2 - (>0.08)     Peak Height 1       essolution Test 2 Pass     Peak Height 1       essolution Test 2 Fail     Peak Height 1	mme     Calc. Type       ssolution Test 1 - (>0.3)     Peak Height with Single E       ssolution Test 1 Fail     Peak Height with Single E       ssolution Test 2 - (>0.00)     Peak Height with Single E       ssolution Test 2 Pass     Peak Height with Single E       esolution Test 2 Pass     Peak Height with Single E       esolution Test 2 Fail     Peak Height with Single E	Imme     Calc. Type       essolution Test 1 - (>0.33)     Peak Height with Single Baseline       essolution Test 1 Fail     Peak Height with Single Baseline       esolution Test 1 Fail     Peak Height with Single Baseline       esolution Test 2 - (>0.08)     Peak Height with Single Baseline       esolution Test 2 Pass     Peak Height with Single Baseline       esolution Test 2 Fail     Peak Height with Single Baseline	ame     Calc. Type     Calc. As       esolution Test 1 < >0.33     Peak Height with Single Baseline     Actual Value       esolution Test 1 Pass     Peak Height with Single Baseline     Actual Value       esolution Test 1 Fail     Peak Height with Single Baseline     Actual Value       esolution Test 2 - (>0.08)     Peak Height with Single Baseline     Actual Value       esolution Test 2 - (>0.08)     Peak Height with Single Baseline     Actual Value       esolution Test 2 Pass     Peak Height with Single Baseline     Actual Value       esolution Test 2 Fail     Peak Height with Single Baseline     Actual Value	ame     Calc. Type     Calc. As     Peak Start       esolution Test 1 - (>0.33)     Peak Height with Single Baseline     Actual Value     2846.5       esolution Test 1 Pass     Peak Height with Single Baseline     Actual Value     2846.5       esolution Test 1 Fail     Peak Height with Single Baseline     Actual Value     2846.5       esolution Test 2 - (>0.08)     Peak Height with Single Baseline     Actual Value     1582       esolution Test 2 Pass     Peak Height with Single Baseline     Actual Value     1582       esolution Test 2 Fail     Peak Height with Single Baseline     Actual Value     1582	Imme     Calc. Type     Calc. As     Peak Start     Peak Stop       ssolution Test 1 < >0.33     Peak Height with Single Baseline     Actual Value     2846.5     2864.5       ssolution Test 1 Pass     Peak Height with Single Baseline     Actual Value     2846.5     2864.5       ssolution Test 1 Fail     Peak Height with Single Baseline     Actual Value     2846.5     2864.5       ssolution Test 2 - (>0.08)     Peak Height with Single Baseline     Actual Value     1582     1588       ssolution Test 2 Pass     Peak Height with Single Baseline     Actual Value     1582     1588       ssolution Test 2 Pass     Peak Height with Single Baseline     Actual Value     1582     1588       ssolution Test 2 Fail     Peak Height with Single Baseline     Actual Value     1582     1588       ssolution Test 2 Fail     Peak Height with Single Baseline     Actual Value     1582     1588	Imme     Calc. Type     Calc. As     Peak Start     Peak Stop     Baseline 1 Start       issolution Test 1 - (>0.33)     Peak Height with Single Baseline     Actual Value     2846.5     2864.5     2867       issolution Test 1 Pasi     Peak Height with Single Baseline     Actual Value     2846.5     2864.5     2867       issolution Test 1 Pai     Peak Height with Single Baseline     Actual Value     2846.5     2864.5     2867       issolution Test 2 - (>0.08)     Peak Height with Single Baseline     Actual Value     1582     1588     1589       issolution Test 2 Pasi     Peak Height with Single Baseline     Actual Value     1582     1588     1589       issolution Test 2 Fail     Peak Height with Single Baseline     Actual Value     1582     1588     1589       issolution Test 2 Fail     Peak Height with Single Baseline     Actual Value     1582     1588     1589	imme     Calc. Type     Calc. As     Peak Start     Peak Stop     Baseline 1 Start     Baselie       esolution Test 1 - (>0.3)     Peak Height with Single Baseline     Actual Value     2846.5     2867.5     2867     2877       solution Test 1 Pas     Peak Height with Single Baseline     Actual Value     2846.5     2864.5     2867     2877       esolution Test 1 Fail     Peak Height with Single Baseline     Actual Value     2846.5     2867.5     2867     2877       esolution Test 2 - (>0.08)     Peak Height with Single Baseline     Actual Value     1582     1588     1589     1594       esolution Test 2 Pas     Peak Height with Single Baseline     Actual Value     1582     1588     1589     1594       esolution Test 2 Fail     Peak Height with Single Baseline     Actual Value     1582     1588     1589     1594       esolution Test 2 Fail     Peak Height with Single Baseline     Actual Value     1582     1588     1589     1594       esolution Test 2 Fail     Peak Height with Single Baseline     Actual Value     1582     1589     1594       Add     Remove     Edit     Edit     Feak Height With Single Baseline     Actual Value     1582     1589     1594

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.

Info	Туре	Instrument	Components (	Comp Reporting	Custom Fields	Recomme	nd Reports		
Name			Calc. Type		Calc. As	Peak Start	Peak Stop	Baseline 1 Start	Baseli Up
Resol	tion Tes	t 1 – (>=18)	Peak Height wi	th Single Baseli	ne Actual Value	2867	2877	2846.5	2854.5
Resol	ition Tes	t 1 Pass	Peak Height wi	th Single Baseli	ne Actual Value	2867	2877	2846.5	2854.5
Resol	uion Tes	t 1 Fail	Peak Height wi	th Single Baseli	ne Actual Value	2867	2877	2846.5	2854.5
Resol	tion Tes	t 2 – (>=12)	Peak Height wi	th Single Baseli	ne Actual Value	1589	1588	1582	1594
Resol	ition Tes	t 2 Pass	Peak Height wi	th Single Baseli	ne Actual Value	1589	1588	1582	1588
Resol	ition Tes	t 2 Fail	Peak Height wi	th Single Baseli	ne Actual Value	1589	1594	1582	1588
Overa	I test res	sult Positive	Peak Height		Actual Value	2867	2877		
									Dov
Ade	l	Remove	Edit						,

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<sup>-1</sup> to the minimum at about 2870 cm<sup>-1</sup> (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<sup>-1</sup> to the minimum at about 1589 cm<sup>-1</sup> (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.

		llsor:	lleer	
		Mothod:		POWER
		wethou.	JF - RESOLVING	
Info	lyp	e Instrume	nt Components Comp Re	porting Custom Fields Recommend Reports
Disp	lay?	Report As	Name	Group Up
		Value	Resolution Test 1 – (>=18)	Test 1: The depth of the trough from the maximum absorption at about 2
		Custom Text	Resolution Test 1 Pass	Measured Accuracy (RESOLVING POWER – Test 1: Outcome)
		Custom Text	Resoltuion Test 1 Fail	Measured Accuracy (RESOLVING POWER – Test 1: Outcome)
		Value	Resolution Test 2 – (>=12)	Test 2: The depth of the trough from the maximum at about 1583 cm-1 t
		Custom Text	Resolution Test 2 Pass	Measured Accuracy (RESOLVING POWER – Test 2: Outcome)
		Custom Text	Resolution Test 2 Fail	Measured Accuracy (RESOLVING POWER – Test 2: Outcome)
		Custom lext	Overall test result Positive	Overall test result
		Custom Text	Overall test result Negative	Overall test result
<				> Down
	Edit			
			Home Save	Save As Methods

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.

User:	User				
Metho	d: JP – RESOLV	ING POWER			
nfo Type Instr	ument Components Co	mp Reporting Custom Fields	Recommend R	eports	
Name	Condition(s)	Recommendation Text			Up
Positive Outcome	"[all_comp]" is Good	All test results are within a	ceptable limits. De	etails given below	
<					> Down
Add Re	emove Edit				
	Home Sav	Save As		Methods	M11
		S			

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 REPRODUCIBILITY" 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.

Info	Type	Instrument	JP - VVAVE Components	Comp Rep	ortino	Custom Fields	Recommend	Reports		
Co	ectral Da	nan (nm 1):	4000	to	85	0				
Sp	ecuarka	nge (cm-r).	4000	10	0.51	0				
	Backgro	und Scans:	140	0						
	Sar	nple Scans:	140							
	Recolu	tion (cm. 1)	4	~		Zero Fill Factor	9			
	resolu	aon (cm-r).	-			Zero i ni ractor.	0			
	1	Apodization:	HappGenzel	~		Phase Correct:	Mertz	~		
9	Sampling	Technology:	Transmission (	Cell	~	Set Method G	ain	Normalize Quant	itative results t	0
						Gain (192-255):	203	Pathlength (µm):	100.0	
	Sampli	ng Subtype:	<any type=""></any>		~					
	Det	ector Type:	<any type=""></any>	1	~					
			Store GPS D	ata						
			Require GPS	S Data						
*	To edit ite	ms on this ta	ab, the user mus	st have Deve	lope	r role rights				

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 <sup>-1</sup> "	Peak Height	3060	-	2
"%T of band at ~2849 cm <sup>-1</sup> "	Peak Height	2849	-	2
"%T of band at ~1601 cm <sup>-1</sup> "	Peak Height	1601	-	2
"%T of band at ~1583 cm <sup>-1</sup> "	Peak Height	1583	-	2
"%T of band at ~1154.5 cm <sup>-1</sup> "	Peak Height	1154.5	-	2
"%T of band at ~1028 cm <sup>-1</sup> "	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<sup>-1</sup> ".
- 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 <sup>-1</sup> "				
"%T of band at ~3060 cm <sup>-1</sup> "	"TRANSMITTANCE REPRODUCABILITY: %T of band at about 3060 cm <sup>-1</sup> "				
"%T of band at ~2849 cm <sup>-1</sup> "	"TRANSMITTANCE REPRODUCABILITY: %T of band at about 2849 cm <sup>-1</sup> "				
"%T of band at ~1601 cm <sup>-1</sup> "	"TRANSMITTANCE REPRODUCABILITY: %T of band at about 1601 cm <sup>-1</sup> "				
"%T of band at ~1583 cm <sup>-1</sup> "	"TRANSMITTANCE REPRODUCABILITY: %T of band at about 1583 cm <sup>-1</sup> "				
"%T of band at ~1154 cm <sup>-1</sup> "	"TRANSMITTANCE REPRODUCABILITY: %T of band at about 1154 cm <sup>-1</sup> "				
"%T of band at ~1028 cm <sup>-1</sup> "	"TRANSMITTANCE REPRODUCABILITY: %T of band at about 1028 cm <sup>-1</sup> "				

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

eport As Name lue Peak Position 3 lue Peak Position 1 lue %T of band at ~	Group 060 WAVE 028.3 WAVE 3060 cm-1 TRAN	NUMBER REPRODU NUMBER REPRODU	CABILITY: Wavenumb	ber Position of band at	Up
lue %T of band at ~ wT of band at ~ lue %T of band at ~ lue %T of band at ~ lue %T of band at ~	2849.5 cm-1 TRAN: 1601.2 cm-1 TRAN: 1583 cm-1 TRAN: 1154.5 cm-1 TRAN: 1028.3 cm-1 TRAN:	SMITTANCE REPROE SMITTANCE REPROE SMITTANCE REPROE SMITTANCE REPROE SMITTANCE REPROE SMITTANCE REPROE	UCABILITY: %T of ba UCABILITY: %T of ba UCABILITY: %T of ba UCABILITY: %T of ba UCABILITY: %T of ba	the result of band at and at about 3060 cm- and at about 2849 cm- and at about 1601 cm- and at about 1683 cm- and at about 1583 cm- and at about 1154 cm- and at about 1028 cm-	1 1 1 1 1 1
				>	Dowr
	ue %T of band at ~ ue %T of band at ~ ue %T of band at ~	µe %T of band at ~1583 cm-1 TRAN: µe %T of band at ~1154.5 cm-1 TRAN: µe %T of band at ~1028.3 cm-1 TRAN:	<ul> <li>%T of band at ~1583 cm-1 TRANSMITTANCE REPROD %T of band at ~1154.5 cm-1 TRANSMITTANCE REPROD we %T of band at ~1028.3 cm-1 TRANSMITTANCE REPROD</li> </ul>	96 WT of band at ~1583 cm-1 TRANSMITTANCE REPRODUCABILITY: %T of band at ~1154.5 cm-1 TRANSMITTANCE REPRODUCABILITY: %T of band at ~1028.3 cm-1 TRANSMITTANCE REPRODUCABILITY: %T of band a	WE of band at ~1583 cm-1 TRANSMITTANCE REPRODUCABILITY: %T of band at about 1583 cm- %T of band at ~1154.5 cm-1 TRANSMITTANCE REPRODUCABILITY: %T of band at about 1154 cm- %T of band at ~1028.3 cm-1 TRANSMITTANCE REPRODUCABILITY: %T of band at about 1028 cm- %T of band at ~1028.3 cm-1 TRANSMITTANCE REPRODUCABILITY: %T of band at about 1028 cm-

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**

4.1 Create/edit a report template	27
4.2 Customize the report template	28
4.3 Assign the report templates to the respective method	30

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.

	-
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

Table 9	Example of MicroLab Reporting Parameters
---------	--

## 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

Test Summary The WAVE NUMBER REPRODUCABILITY and TRANSMITTANCE REPRODUCABILITY test in ac Pharmacopeia (JP XVII) consists of two measurements. The results of these two measurements (R are used to manually calculate the relevant test criteria. A record of Run 1 and Run 2 is considered a documentation of the test outcome. <u>Test Details</u>	c. to Japanese ın 1 and Run 2) sufficient as
Specification	Result
ComponentName	Result
Verification of WAVE NUMBER REPRODUCABILTY  - Perform two runs and calculate the difference of the Wavenumber Positions found in F - A calculated difference of - 5 cm <sup>-1</sup> for the band at about 3006 cm <sup>-1</sup> - 4 cm <sup>-1</sup> for the band at about 1028 cm <sup>-1</sup> is considered validation of the WAVE NUMBER REPRODUCABILTY.	tun 1 and Run 2
Verification of TRANSMITTANCE REPRODUCABILTY	
<ul> <li>Perform two runs and calculate the difference of the %T found in Run 1 and Run 2         <ul> <li>A calculated difference of </li> <li>0.5 %T</li> <li>is considered validation of the TRANSMITTANCE REPRODUCABILTY.</li> </ul> </li> </ul>	
Note: The full instrument performance validation consists of three Parts. Part 1: WAVE NUMBER SCALE Part 2: RESOLVING POWER Part 3: WAVE NUMBER REPRODUCABILITY and TRANSMITTANCE REPRODUCABILI (Run 1 and Run 2)	TY
4/1/2024 10:23:58 PM	page 2 of 3

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

а

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.

User:	User
Method	: JP - WAVE NUMBER SCALE
Info Type Instrum	nent Components Comp Reporting Custom Fields Recommend Reports
Available Report Templa	ates: Selected Report Templates:
	<- Remove
Results Folder:	<- Remove
Results Folder: Auto-Export :	<- Remove
Results Folder: Auto-Export : Results Naming:	<- Remove
Results Folder: Auto-Export : Results Naming: Sample ID	<- Remove All Selected Reports
Results Folder: Auto-Export : Results Naming: Sample ID @ Date Time	<- Remove Auto-Report All Selected Reports <no auto-export="">   + increment (Sample ID required)</no>
Results Folder: Auto-Export : Results Naming: Sample ID @ Date Time Sample ID	<- Remove Auto-Report All Selected Reports <no auto-export="">   + increment (Sample ID required)   + Date Time</no>
Results Folder: Auto-Export : Results Naming: Sample ID Sample ID Sample ID	<- Remove All Selected Reports  Auto-Report All Selected Reports  * No Auto-Export>  * increment (Sample ID required)  * Date Time

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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5.4 Perform the Wave Number Reproducibility and Transmittance Reproducibility test	36

### 5.1 Preparing the Cary 630 FTIR

- 1 Connect the Cary 630 FTIR to the PC and switch it on.
- 2 Start MicroLab PC.

5

**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**.

MicroLab			_ =	
MicroLab	Unan	User		
O Status: Resolv	Method:	JP - WA	AVE NUMBER SCALE	
Prepare sample	_	then	close compartment	I
Home			Next >	
		Ag	ilent Technologies	

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.

Us	er:	User			
Re	sult:	2024-06-04T15-46-00			
Recommendation	:				
All test results a	ire withir	acceptable limits. Details given below			
(esults:					
lame			Value	Low Threshold	High Threshold
Aeasured Peak Po	sition (Sp	ec. WN: 1028.3 cm-1)	1028.3	1027.3	1029.4
Measured Accuracy (Peak at 1028.3 cm-1, Spec. Acc.: +-1 cm-1)			0.0	-1	1.1
Measured Peak Position (Spec. WN: 1154.5 cm-1)			1154.5	1153.5	1155.6
Measured Accuracy (Peak at 1154.5 cm-1, Spec. Acc.: +-1 cm-1)			0.0	-1	1.1
Measured Peak Position (Spec. WN: 1583 cm-1)			1583.0	1582	1584.1
Measured Accuracy (Peak at 1583 cm-1, Spec. Acc.: +-1 cm-1)			0.0	-1	1.1
Accounted Peak Po:	Sition (Sp	ec. vvv. 1601.2 cm-1)	1601.0	1000.2	1002.3
Annoured Peak Per	ition (So	ac WN: 2849.6 cm 1)	-0.2	2949	2951.1
Appeured Accuracy	(Dook of	2849.5 cm 1. Spac. Acc : + 1.5 cm 1)	0.2	1.5	1.6
Accuracy Accuracy	tition (So	ac WN: 3060 cm.1)	3059.6	3058.5	3061.6
Accuracy	(Peak at	: 3060 cm-1 Spec Acc : +-1.5 cm-1)	-0.4	-15	16
Verall Test Result	(r ourra		PASS	1	

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.

MicroLab			_ =
O Status: Ready	User: Method:	User JP - RES	OLVING POWER
Prepare compartment for background		then	close compartment
Home			Next >
		Agi	lent Technologies

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.

Us	er:	User	
Re	sult:	2024-04-23T16-27-17	
Recommendation			
All test results a	are within	acceptable limits. Details given below	
Results:			
Name			Value
Test 1: The denth of	f the trough	from the maximum absorption at about 2850 cm.1 to the minimum at about 2870 cm.1 (acceptance criterium $>=$ 18%)	24.61
Measured Accuracy	(RESOLV	(ING POWER – Test 1: Outcome)	Pass
	(· · · · · · · · · · · · · · · · · · ·		
Test 2: The depth of	the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%)	15.07
Test 2: The depth of Measured Accuracy	f the trough (RESOLV	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) //NG POWER – Test 2: Outcome)	15.07 Pass
Test 2: The depth of Measured Accuracy Overall test result	f the trough / (RESOLV	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) (ING POWER – Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough / (RESOLV	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) ING POWER – Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough / (RESOLV	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) ING POWER – Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough (RESOLV	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) ING POWER – Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) (ING POWER − Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) ING POWER – Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) ING POWER – Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) (ING POWER − Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) (ING POWER − Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) (ING POWER – Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) ING POWER – Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	n from the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%) (ING POW/ER − Test 2: Outcome)	15.07 Pass PASS
Test 2: The depth of Measured Accuracy Overall test result	f the trough	If Nom the maximum at about 1583 cm-1 to the minimum at about 1589 cm-1 (acceptance criterium >=12%)         ING POWER - Test 2: Outcome)         Home       Data         Home       Data         Handling       Details	15.07 Pass PASS

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 REPRODUCIBILITY" 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.

O MicroLab			_ 🗷	
MicroLab				
	User:	User		
Status: Receiv	Method:	JP – W	AVE NUMBER REPRODUCIBILITY	
Prepare compartment for background		then	close compartment	
Home			Next >	
		A	jilent Technologies	

Figure 27. Method start screen.

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

9 MicroLab			_ 🗷
MicroLab			
O Status: Greedy	User: Method:	User JP - WA	VE NUMBER REPRODUCIBILITY
Prepare sample	then		close compartment
Home			Next >
		Ag	ilent Technologies

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.

	User:	User			
O Status: Ready	Method:	JP – WAVE N	UMBER REF	PRODUCIBIL	ITY
Recommendation:					
The WAVENUMBER REPRODUCIBILI	TY and TRANSMISSION	REPRODUCIBILITY	test consists of tw	vo measurement	s. The results of
these two measurements (Run 1 and F	Run 2) are used to manu	ally calculate the rele	vant test results a	nd compared aga	inst the limits
Results:					
lame			Value	Low Threshold	High Threshold
WAVE NUMBER REPRODUCABILITY: Wave	number Position of band at	about 3060 cm-1	3059.7		
VAVE NUMBER REPRODUCABILITY: Wave	number Position of band at	about 1028 cm-1	1028.3		
RANSMITTANCE REPRODUCABILITY: %T of	of band at about 3060 cm-1		5.74		
RANSMITTANCE REPRODUCABILITY: %T of	of band at about 2849 cm-1		12.89		
RANSMITTANCE REPRODUCABILITY: %T	of band at about 1601 cm-1		10.66		
RANSMITTANCE REPRODUCABILITY: %T of	of band at about 1583 cm-1		43.60		
RANSMITTANCE REPRODUCABILITY: %1 (	of band at about 1154 cm-1		48.48		
RANSMITTANCE REPRODUCABILITY: %10	of band at about 1028 cm-1		20.47		

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<sup>-1</sup>:

Wavenumber Position of band at about 3060 cm<sup>-1</sup>:

TRANSMITTANCE REPRODUCIBILITY:

%T of band at about 3060 cm<sup>-1</sup>:

%T of band at about 2849 cm<sup>-1</sup>:

%T of band at about 1601 cm<sup>-1</sup>:

%T of band at about 1583 cm<sup>-1</sup>:

%T of band at about 1154 cm<sup>-1</sup>:

%T of band at about 1028 cm<sup>-1</sup>:"

**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 <sup>-1</sup>				<5 cm <sup>-1</sup>	
Wavenumber Position of band at about 1028 cm <sup>-1</sup>				<1 cm <sup>-1</sup>	
TRANSMITTANCE REPRODUCIE	BILITY				
%T of band at about 3060 cm <sup>-1</sup>					
%T of band at about 2849 cm <sup>-1</sup>				_	
%T of band at about 1601 cm <sup>-1</sup>				-0.5%	
%T of band at about 1583 cm <sup>-1</sup>				- <0.5%	
%T of band at about 1154 cm <sup>-1</sup>				-	
%T of band at about 1028 cm <sup>-1</sup>				-	

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

This information is subject to change without notice.



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