

SPECTRUM TWO



User's Guide



DISTRIBUTED BY:

Sedulitas

PEOPLE | PASSION | PRECISION

info@sedulitas.co.za +27 (0)82 551 4001
www.sedulitas.co.za

Release History

Part Number	Release	Publication Date
L1050228	E	November 2012

Any comments about the documentation for this product should be addressed to:

User Assistance
PerkinElmer Ltd
Chalfont Road
Seer Green
Beaconsfield
Bucks HP9 2FX
United Kingdom

Or emailed to: info@perkinelmer.com

Notices

The information contained in this document is subject to change without notice.

Except as specifically set forth in its terms and conditions of sale, PerkinElmer makes no warranty of any kind with regard to this document, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose.

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

Copyright Information

This document contains proprietary information that is protected by copyright.

All rights are reserved. No part of this publication may be reproduced in any form whatsoever or translated into any language without the prior, written permission of PerkinElmer, Inc.

Copyright © 2012 PerkinElmer, Inc.

Trademarks

Registered names, trademarks, etc. used in this document, even when not specifically marked as such, are protected by law.

PerkinElmer is a registered trademark of PerkinElmer, Inc.

AssureID, Spectrum and Spectrum Two are trademarks of PerkinElmer, Inc.

Silver Gate is a trademark of Specac.

MIRacle ATR is a trademark of Pike Technologies.

Contents

Introduction	5
About This Manual	6
Conventions Used in this Manual	7
Notes, Cautions and Warnings.....	7
Warnings and Safety Information	11
Overview	12
Safety Summary.....	13
General Safety	14
Electrical safety	14
Optical radiation	15
Location and Ventilation	16
To allow for adequate cooling	16
To allow any nitrogen used to disperse	16
Use of flammable solvents and samples	16
Warning Signs on the Instrument.....	17
EMC Compliance	18
European EC Directive	18
FCC rules and regulations.....	18
An Overview of the Spectrum Two	19
A Guided Tour of the Spectrum Two.....	20
Optical system.....	21
Sample compartment.....	21
Power switch and communication ports	23
Portability.....	23
Accessories	24
Applications Packs	26
Introductory and Resource Packs.....	26
Analysis Packs	26
Unpacking and Installation	27
Requirements	28
Electrical requirements.....	28
Environment.....	28
Specifications	29
Unpacking the Spectrometer	30
Opening the shipping container	30
Choosing Your Connection Method	32
Installing your Spectrum Two	34
Connecting the spectrometer to the electrical supply	35
Connecting the spectrometer to the PC using the USB cable.....	36
Connecting the spectrometer to the PC using the wireless router.....	38
Connecting the spectrometer to the PC using an Ethernet cable	41
Connecting the spectrometer via a network.....	42
Instrument Install Wizard.....	44
Changing the Sampling Accessory	45
Moving the Spectrometer	48
Getting Started with Spectrum Software	49
Overview	50
Starting Spectrum Software	51
The Spectrum Workspace	53
Using the Spectrum on-screen Help system	56
Scanning Samples	57
Quality Checks	59

Processing Spectra	61
Spectral correction	61
Identification	62
Quantification	66
Macros	70
Scanalyze	71
Saving Spectra, Exporting Spectra and Reporting	72
Saving spectra	72
Exporting spectra	73
Send To	75
Reporting	76
Printing	77
Instrument Settings	78
Changing the Resolution	79
Component Checks	81
Humidity Shield	83
Power Save Mode	85
Using the button on the front of the instrument	85
Using Power Save Mode in Spectrum software	86
Ready Checks and Instrument Verification	87
Atmospheric (CO ₂ /H ₂ O) Suppression	90
AVI Correction	91
AVI Calibration	92
Exit Spectrum Software	93
Maintenance.....	95
Overview.....	96
Cleaning the Spectrometer	97
Changing the Desiccant.....	98
Purging the Spectrometer	101
Purging the sample compartment.....	102
Purging the instrument.....	103
Replacing the Source	106
Installing/Replacing Windows	108
Replacing the Main Board Air Filter	110
Additional Parts	113
Optional parts.....	113
Replacement parts	114
Upgrades.....	114
Appendices.....	115
Appendix 1: Connector Details.....	116
Appendix 2: Instrument Performance Validation Kits.....	117
Appendix 3: Decontamination and Cleaning.....	118
Appendix 4: WEEE Instructions for PerkinElmer Products	119
Index.....	120

Introduction

About This Manual

This manual provides instructions for the installation, use and maintenance of the Spectrum Two spectrometer. It contains the following sections:

- Introduction
- Warnings and Safety Information
- An Overview of the Spectrum Two
- Unpacking and Installation
- Getting Started with Spectrum Software
- Maintenance
- Appendices.

NOTE: This manual shows details for using your instrument with the Spectrum software package (version 10.3 or later). If you have Spectrum ES or AssureID software, please refer to the Administrator's Guide for your software, which can be found on the *Spectrum Two Manuals CD* (part number L1050242), or refer to the on-screen Help.

For further information on collecting, viewing and processing spectra using Spectrum software, refer to the help file that you can access from the Help menu, or by clicking **Help** on a dialog.

Conventions Used in this Manual

Normal text is used to provide information and instructions.

Bold text refers to text that is displayed on the screen.

UPPERCASE text, for example ENTER or ALT, refers to keys on the PC keyboard. "+" is used to show that you have to press two keys at the same time, for example, ALT+F.

All eight-digit numbers are PerkinElmer part numbers unless stated otherwise.

The term "instrument" refers to either the Spectrum Two FT-IR spectrometer, and any sampling accessory fitted.

Notes, Cautions and Warnings

Three terms, in the following standard formats, are also used to highlight special circumstances and warnings.

NOTE: A note indicates additional, significant information that is provided with some procedures.



WARNING

We use the term **WARNING** to inform you about situations that could result in **personal injury** to yourself or other persons. Details about these circumstances are in a box like this one.

D

Warning (Warnung)

Bedeutet, daß es bei Nichtbeachten der genannten Anweisung zu einer **Verletzung** des Benutzers kommen kann.

DK

Warning (Advarsel)

Betyder, at brugeren kan blive **kvæstet**, hvis anvisningen ikke overholdes.

E

Warning (Peligro)

Utilizamos el término **WARNING (PELIGRO)** para informarle sobre situaciones que pueden provocar **daños personales** a usted o a otras personas. En los recuadros como éste se proporciona información sobre este tipo de circunstancias.

F

Warning (Danger)

Nous utilisons la formule **WARNING (DANGER)** pour avertir des situations pouvant occasionner des **dommages corporels** à l'utilisateur ou à d'autres personnes. Les détails sur ces circonstances sont donnés dans un encadré semblable à celui-ci.

I

Warning (Pericolo)

Con il termine **WARNING (PERICOLO)** vengono segnalate situazioni che potrebbero provocare **incidenti alle persone**. Troverete informazioni su tali circostanze in un riquadro come questo.

NL

Warning (Waarschuwing)

Betekent dat, wanneer de genoemde aanwijzing niet in acht wordt genomen, dit kan leiden tot **verwondingen** van de gebruiker.

P

Warning (Aviso)

Significa que a não observância da instrução referida poderá causar um **ferimento** ao usuário.

CN

Warning (警告)

我们使用“警告”这一术语来通知您有关可能会对您自己或他人造成人身伤害的情况。

有关这些情况的详细信息可在此类方框中找到。

JP

Warning (警告)

使用者及びその他周辺に危害が及ぶ恐れがある場合は、この様なボックスの中に注意事項が表示されています。

CAUTION

We use the term **CAUTION** to inform you about situations that could result in **serious damage to the instrument** or other equipment. Details about these circumstances are in a box like this one.

D**Caution (Achtung)**

Bedeutet, daß die genannte Anleitung genau befolgt werden muß, um einen **Gerüteschaden** zu vermeiden.

DK**Caution (Bemærk)**

Dette betyder, at den nævnte vejledning skal overholdes nøje for at undgå en **beskadigelse af apparatet**.

E**Caution (Advertencia)**

Utilizamos el término **CAUTION (ADVERTENCIA)** para advertir sobre situaciones que pueden provocar **averías graves en este equipo** o en otros. En los recuadros como éste se proporciona información sobre este tipo de circunstancias.

F**Caution (Attention)**

Nous utilisons le terme **CAUTION (ATTENTION)** pour signaler les situations susceptibles de provoquer de **graves détériorations de l'instrument** ou d'autre matériel. Les détails sur ces circonstances figurent dans un encadré semblable à celui-ci.

I**Caution (Attenzione)**

Con il termine **CAUTION (ATTENZIONE)** vengono segnalate situazioni che potrebbero arrecare **gravi danni allo strumento** o ad altra apparecchiatura. Troverete informazioni su tali circostanze in un riquadro come questo.

NL**Caution (Opgelet)**

Betekent dat de genoemde handleiding nauwkeurig moet worden opgevolgd, om **beschadiging van het instrument** te voorkomen.

P**Caution (Atenção)**

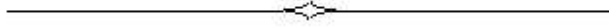
Significa que a instrução referida tem de ser respeitada para evitar a **danificação do aparelho**.

CN**Caution (小心)**

我们使用“小心”这一术语来通知您有关可能会对**本仪器或其它设备造成严重损害**的情况。
有关这些情况的详细信息可在此类方框中找到。

JP**Caution (注意)**

分光器や他の機材等に深刻なダメージを与える恐れがある場合は、この様なボックスの中に表示しています。



Warnings and Safety
Information

Overview

This chapter describes the general safety practices and precautions that must be observed when operating the Spectrum Two FT-IR spectrometer.

This advice is intended to supplement, not supersede, the normal safety codes in the user's country. It is also a supplement to the PerkinElmer standard Safety and Health Policy. The information provided does not cover every safety procedure that should be practiced. Ultimately, maintenance of a safe laboratory environment is the responsibility of the analyst and the analyst's organization.

Please consult all manuals supplied with the Spectrum Two and accessories before you start working with the instrument. Carefully read the safety information in this chapter and in the other manuals supplied. When setting up the instrument or performing analyses or maintenance procedures, strictly follow the instructions provided.

Safety Summary

The Spectrum Two FT-IR spectrometers have been designed to comply with a wide variety of international standards governing the safety of laboratory equipment. In routine use, the instruments pose virtually no risk to you. If you take some simple, common-sense precautions, you can make sure that you maintain the continued safe operation of your instrument:

- DO make sure that the power supply is properly connected to the electrical supply; in particular make sure that the ground (earth) is securely connected.
- DO disconnect the electrical power cable before opening any ports or covers on the instrument, unless otherwise directed in the maintenance procedures described in this manual, or in Spectrum, Spectrum ES or AssureID software.
- DO NOT open the main instrument cover. There are no user-serviceable parts inside the main cover, and tampering with the seal will invalidate your warranty.
- DO keep the instrument dry. Avoid spilling liquid onto the instrument. Clean all external spills immediately.
- DO NOT use a flammable gas to purge the instrument. The instrument contains a hot source, and a fire or explosion will result. Only use clean, dry, oil-free nitrogen or air to purge the instrument.
- DO read the more detailed information on warnings and safety in the following pages to ensure the safe operation of the instrument.

General Safety

The Spectrum Two FT-IR spectrometers have been designed and tested in accordance with PerkinElmer specifications and in accordance with the safety requirements of the International Electrotechnical Commission (IEC). The instruments conform to IEC publication 61010-1 ("Safety requirements for electrical equipment for measurement, control, and laboratory use") and therefore meets the requirements of EC low voltage directive 2006/95/EC.

If the instrument is used in a manner not specified by the manufacturer, the protection provided by the instrument may be impaired. Only use the instrument under the following environmental conditions:

Temperature	0 °C to 50 °C
Relative Humidity	90% maximum (non-condensing)



WARNING

If the equipment is used in a manner not specified herein the protection provided by the equipment may be impaired.

Electrical safety

- Connect the instrument power supply to a power outlet that includes a switch or other means of disconnection from the electricity supply.
- Only plug the instrument power supply into a socket power outlet that is provided with a protective earth connection.
- The instrument must be disconnected from all voltage sources before it is opened for any adjustment, replacement, maintenance or repair, unless otherwise directed in the maintenance procedures described in this manual, or in Spectrum, Spectrum ES or AssureID software.



WARNING

To ensure safe and satisfactory operation of the instrument, it is essential that the green or green/yellow ground (earth) wire of the power cord is connected to a ground that complies with the regulations of the local electricity supply authority (or equivalent body); ground circuit continuity is essential for safe operation of the equipment.

Only connect equipment that meets the requirements of IEC 61010-1, IEC 60950 or equivalent standards.

The power supply adaptor has been designed to be safe under the following environmental conditions:

- Indoor use
- Altitude up to 2000 m (above mean sea level)
- Ambient temperatures of 0 °C to 50 °C
- Mains supply fluctuations not exceeding $\pm 10\%$ of the nominal voltage.

If it is necessary to fit a plug on the power cable supplied, use the wire color code below:

Plug Pin	Wire Color (100–120 V)	Wire Color (220–240 V)
Ground (Earth)	Green or Green/Yellow	Green/Yellow
Live	Black	Brown
Neutral	White	Blue

Optical radiation

The instrument complies with the requirements of the Artificial Optical Radiation Directive 2006/25/EC.

Location and Ventilation

To allow for adequate cooling

- Do not site the instrument near to room-heating equipment, for example, central-heating radiators.
- Do not block the ventilation cooling holes under the instrument.
- Do not cover the power supply adaptor.

To allow any nitrogen used to disperse



Do not site the instrument in a poorly ventilated area if nitrogen will be used as a purge gas.

Oxygen depletion in an enclosed space does not trigger a gasping reflex, and errors of judgment, confusion, or unconsciousness can occur in seconds and without warning.

The spectrometer has a connector that enables the sample compartment to be purged using clean, dry, oil-free air or nitrogen. The recommended flow rate is 4 L/min. It also has two connectors that enable the instrument body to be purged. The recommended flow rate is 2 L/min.

The sample compartment purge vents to its surroundings. The instrument purge outlet can be connected with tubing to vent outside the working environment, for example to a fume cabinet.

Use of flammable solvents and samples



The instrument contains a hot source, and contact with flammable vapors may cause an explosion. Flammable solvents or samples should not be stored on or near the instrument. During sample preparation, such materials should be handled in a safe area away from the instrument, such as a fume cabinet.

Warning Signs on the Instrument

	<p><i>Warning.</i></p> <p><i>Refer to accompanying documents in all cases where this symbol is used to find out the nature of the potential hazard and any actions which have to be taken.</i></p>
--	----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

A warning label is attached to the source compartment (Figure 1). Refer to *Replacing the Source* on page 106.



Figure 1 Labels (rear of instrument)

A warning label is attached to the desiccant compartment and near the instrument purge inlet port (Figure 2). Refer to *Changing the Desiccant* on page 98 or to *Purging the instrument* on page 103, as applicable.

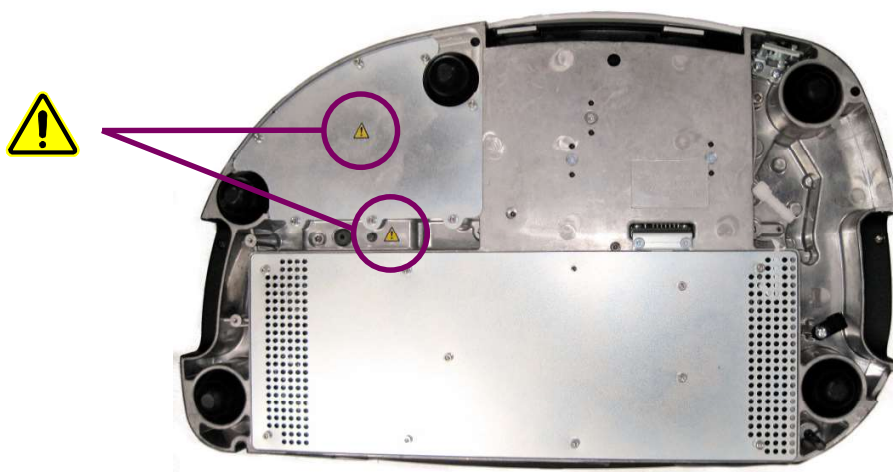


Figure 2 Labels (base of instrument)

EMC Compliance

European EC Directive

The Spectrum Two spectrometers have been designed and tested to meet the requirements of the EC Directive 2004/108/EC.

FCC rules and regulations

These products are classified as digital devices used exclusively as industrial, commercial, or medical test equipment. They are exempt from the technical standards specified in Part 15 of the FCC Rules and Regulations, based on Section 15.103(c).

An Overview of the **Spectrum Two**

A Guided Tour of the Spectrum Two

PerkinElmer Spectrum Two spectrometers are compact, robust instruments that can be used in non-laboratory environments.



Figure 3 Spectrum Two Spectrometer

- Spectrum Two FT-IR spectrometers with standard detector:
 - Standard, high-performance, room-temperature LiTaO₃ (lithium tantalate) MIR detector.
 - Optical system with KBr windows enables you to collect data over a total range of 8300 to 350 cm⁻¹ at a best resolution of 0.5 cm⁻¹.
 - Optional ZnSe windows, for use in exceptionally humid environments, enable data collection over a range of 6000 to 550 cm⁻¹ at a best resolution of 0.5 cm⁻¹.
 - Optional APV/AVI configuration.

For APV, an internal, software-controlled filter wheel comes complete with traceable reference materials for automatic performance verification. Also, the methane cell provided enables the production of standard data to be referenced to fundamental band positions using the Absolute Virtual Instrument (AVI) feature.

- Spectrum Two FT-IR spectrometers with temperature-stabilized detector:
 - Temperature-stabilized, high-performance, DTGS (deuterated triglycine sulphate) MIR detector for enhanced signal-to-noise.
 - Optical system enables you to collect data over a total range of 8300 to 350 cm⁻¹ at a best resolution of 0.5 cm⁻¹ with KBr windows.
 - Optional ZnSe windows, for use in exceptionally humid environments, enable data collection over a range of 6000 to 550 cm⁻¹ at a best resolution of 0.5 cm⁻¹.
 - Optional APV/AVI configuration.

For APV, an internal, software-controlled filter wheel comes complete with traceable reference materials for automatic performance verification. Also, the methane cell provided enables the production of standard data to be referenced to fundamental band positions using the Absolute Virtual Instrument (AVI) feature.

The instrument is connected to a PC, either point-to-point (USB 2.0 or Ethernet), over a network, or via a wireless network using the optional wireless router.

The Spectrum software supplied enables you to control the instrument and to manipulate the spectra that you collect. The spectrometers can operate in ratio, single-beam, or interferogram mode.

Optical system

The optical system is under the main cover of the instrument. The instrument is sealed at the factory, and the main cover of the instrument should not be opened.

No panel of the spectrometer should be removed unless following the maintenance procedures described in this manual. In particular, maintenance procedures that risk ingress of water vapor into the instrument should be performed only using the appropriate maintenance wizard in Spectrum, Spectrum ES or AssureID Software. See *Maintenance* on page 95 for more information.

Stability of the optical system

The system is purged and sealed at the factory. A supply of desiccant placed within the system removes any water vapor and carbon dioxide that may enter. The unique humidity shield design (part of the OpticsGuard™ system) protects the spectrometer from environmental conditions, meaning it can be used in more challenging environments. In addition, the internal humidity sensor, in conjunction with the Humidity Shield feature in Spectrum software, warns you when the desiccant needs changing. Refer to *Humidity Shield* on page 83 for further information.

In the Spectrum Two FT-IR spectrometer, KBr or ZnSe windows separate the sample compartment from the purged optical system.

You can purge the sample compartment with clean, dry, oil-free air or nitrogen. Either one removes water vapor; however, nitrogen is preferable because it also removes atmospheric carbon dioxide.

Sample compartment

The instrument has a versatile, purgeable sample compartment (Figure 4) located at the front of the instrument. Open the sample compartment by lifting the cover using the recess at the front.

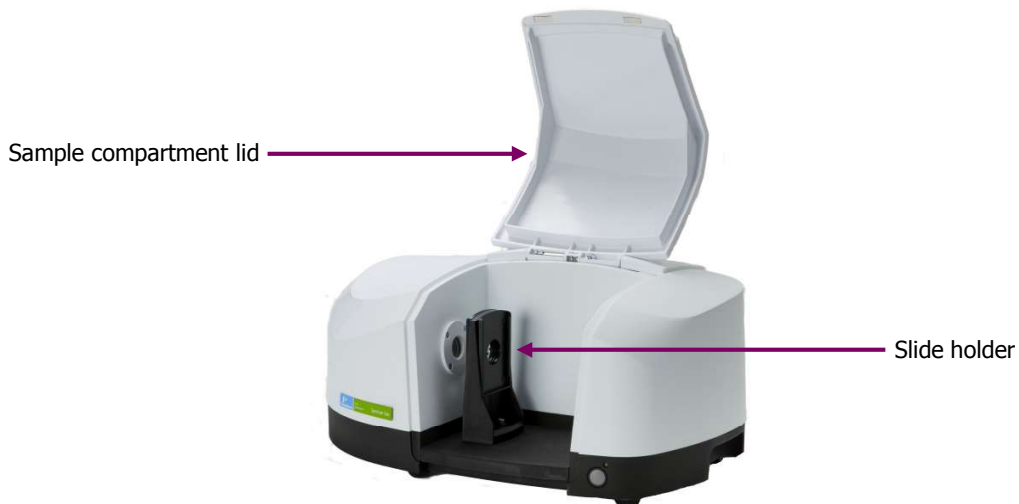


Figure 4 Sample compartment

The infrared beam enters the sample compartment through a window on the left. After passing through the sample, it enters the detector area through a window on the right side of the sample compartment.

CAUTION

The KBr sample compartment windows fitted in some Spectrum Two FT-IR spectrometers, although coated to prevent damage by small amounts of condensation, may be damaged by large amounts of condensation build-up in the rim of the windows.

Take care not to scratch the windows when installing accessories or using sample tools.

Standard accessories are mounted on a baseplate. The standard baseplate has a slide holder that can be fitted at two positions, fixed by a single screw (Figure 5).



Figure 5 Slide holder on standard baseplate

The slide holder has two slide positions that enable you to insert a sample and a J-stop card for measurements at high resolutions.

For more information on using the J-stop cards, see *Changing the Resolution* on page 79.

Power switch and communication ports

The DC power connector and communication ports are on the rear of the instrument.

The Power on LED on the front of the instrument will light green when the instrument is connected to mains power and is switched on (Figure 6).



Figure 6 Power ON LED

NOTE: The Spectrum Two spectrometer is usable within 15 minutes of being switched on after being switched off overnight. However, if your instrument has recently been transferred from a much colder environment, it is advisable to run a background spectrum before every sample for the first couple of hours of use.

Portability

The compact and robust design of the Spectrum Two means that the instrument can be easily transferred between environments. The simple user-installation, and fast warm-up time, means that the instrument can be set up quickly. The range of accessories available help you to move your analysis out of the laboratory. Optional wireless connectivity enables portable PC control, and the multiple power options enable you to use your spectrometer with, or without, external mains power (Figure 7).



Figure 7 Spectrum Two with wireless router and battery pack

NOTE: The battery pack can also be used as an uninterruptable power supply (UPS).

The Portability Pack includes a battery pack and 12 V car auxiliary port adaptor, spectrometer carry case and a wireless router kit. The individual components of the Portability Pack are also available separately. Refer to *Optional parts* on page 113.

Accessories

There is a range of optional sampling accessories available for the Spectrum Two FT-IR spectrometer that fit in the sample compartment, including:

- Spectrum Two Universal ATR (Single Reflection Diamond) – L1600107
The universal ATR is a general accessory for the analysis of solids and liquids. The pressure arm enables good contact of the sample with the diamond crystal (Figure 8). Refer to the *Spectrum Two UATR User's Guide* (part number L1050231) available as a pdf on the *Spectrum Two Manuals CD* (part number L1050242) for information on using the accessory.



Figure 8 Spectrum Two FT-IR with Universal ATR Accessory

- Spectrum Two HATR (ZnSe Flat Plate) – L1600113
The accessory is supplied with a flat top-plate fitted with a 25-reflection, 45-degree, 50-mm ZnSe crystal, enabling simple sampling of solids, polymer films and powders. Additional top plates with germanium, AMTIR-1 and KRS-5 crystals are also available. Refer to the *Spectrum Two HATR User's Guide* (part number L1050232) available as a pdf on the *Spectrum Two Manuals CD* (part number L1050242) for information on using the accessory.
- Spectrum Two HATR (ZnSe Trough Plate) – L1600109
The accessory is supplied with a trough plate fitted with a 25-reflection, 45 degree, 50-mm ZnSe crystal, allowing easy sampling of liquids, pastes and gels. Additional top plates with germanium, AMTIR-1 and KRS-5 crystals are also available. Refer to the *Spectrum Two HATR User's Guide* (part number L1050232) available as a pdf on the *Spectrum Two Manuals CD* (part number L1050242) for information on using the accessory.
- Spectrum Two Diffuse Reflectance Accessory – L1600111
The Diffuse Reflectance Accessory provides a solution for analyzing opaque or highly scattering solid samples such as pharmaceuticals, food products, soap powders, coal, clay, soil, paper, painted surfaces, polymer foam and catalysts. Refer to the *Spectrum Two Diffuse Reflectance Accessory User's Guide* (part number L1050233) available as a pdf on the *Spectrum Two Manuals CD* (part number L1050242) for information on using the accessory.

- Fixed Angle Specular Reflectance (FASR) Accessory (16°) – L1600119
The FASR Accessory enables you to obtain a spectrum of any flat, reflecting surface on plate or sheet material; for example, thin coatings on metal surfaces, such as drink cans. One mirror focuses the IR beam at the sample; the other collects the reflected radiation. The accessory is supplied with a reference mirror that is used to obtain reference spectra.
The FASR accessory is mounted using the slide holder.
Refer to the *Spectrum Two Fixed Angle Specular Reflectance Accessory User's Guide* (part number L1050234) available as a pdf on the *Spectrum Two Manuals CD* (part number L1050242) for information on using the accessory.

It is easy to remove an accessory and replace it with another. Refer to *Changing the Sampling Accessory* on page 45. For the baseplate-mounted accessories, a coded connector on the baseplate plugs into a socket on the rear wall of the sample compartment. The instrument identifies the type of accessory and automatically updates the instrument settings.

NOTE: Several third-party accessories are also available for the Spectrum Two, including the Pike MIRacle ATR and the Specac Sliver Gate ATR. Those pre-mounted on a baseplate will also be recognized by the Spectrum software, and details of the accessory will be stored in the header information of any spectra collected.

Contact your PerkinElmer Customer Care Representative for more information.

Gas cells with NaCl, KBr or CaF₂ windows are available. You will require the universal gas cell mount (10 cm), which is inserted into the slide holder.

NOTE: For slide-holder mounted accessories, you can select a **Sampling** option from the drop-down list on the Setup Instrument basic tab in Spectrum software.

Applications Packs

You can purchase a number of packs designed to help you with specific application areas.

Introductory and Resource Packs

Part Number	Description
L1608001/ L1608002	FT-IR Introductory Kit (1 User/5 Users)
L1608003	FT-IR Educational Resource Pack
L1608004	FT-IR Pharmacopoeia Compliance Resource Pack
L1608005	FT-IR Nutraceutical Compliance Resource Pack
L1608013	FT-IR Polymer Resource Pack

Analysis Packs

The Analysis packs include accessories, consumables and Spectrum Touch™ software.

Part Number	Description
L1608006	Environmental Hydrocarbon ASTM D7066 Analysis Pack
L1608007	Environmental Hydrocarbon Cyclohexane Analysis Pack
L1608008	Environmental Hydrocarbon ATR Analysis Pack (includes HATR Accessory)
L1608009	In-Service Lubricants Analysis Pack
L1608010	FT-IR Biodiesel Analysis Pack
L1608012	FT-IR Benzene In Gasoline Analysis Pack
L1608015	<i>trans</i> Fat FT-IR Analysis Pack

Unpacking and **Installation**

Requirements

NOTE: Read the warnings and safety information chapter in this manual before you install the instrument. It contains important information.

Electrical requirements

The Spectrum Two power supply adaptor can operate on electricity supplies of 50 or 60 Hz and in the 100 to 230 V range without any adjustment.

The maximum power consumption of the system is 65 VA (approximately 40 W) when powering the wireless router. In Power Save mode the mains power consumption is <10 VA (approximately 6 W) and the DC power consumption is 0.2 W.

The line supply must be within 10% of the nominal voltage.

If possible, do not connect the instrument to circuits that have heavy-duty equipment connected, such as large motors.

If possible, do not use photocopiers, discharge lamps, radio transmitters, and other equipment with large or frequent transient loads on the same supply circuit.

Environment

To obtain the best performance from your instrument:

- Place the instrument in an environment that is relatively dry and dust-free.
- Make sure that the bench top is free from vibration or mechanical shocks.
- Do not place the instrument or the PC near to room-heating equipment, such as central-heating radiators.
- Do not position the instrument in direct sunlight as this may cause overheating.
- Ensure that there is sufficient clearance underneath the instrument to permit an adequate flow of cooling air.
- The area near the PC must be free of strong magnetic fields, direct sunlight, and heating or cooling units or ducts.

Specifications

Specification	Value
Dimensions	450 × 300 × 210 mm (<i>W × D × H</i>) 450 × 300 × 300 mm with UATR installed
Weight	Approximately 13 kg
Power input	100–230 V, 50/60 Hz, Max 65 VA
Laser	Class 1
Detector	DTGS or LiTaO ₃
Operating temperature range	0 °C to 50 °C*
Storage temperature range	–20 °C to 60 °C
Maximum relative humidity	80% (non-condensing) with KBr windows 90% (non-condensing) with ZnSe windows

* If you intend to operate your instrument regularly at temperatures of 40 °C or higher, for optimum performance we recommend that you repeat the Wavelength Calibration at the appropriate operating temperature. Refer to the on-screen help for your software application.

Unpacking the Spectrometer

CAUTION

Take great care when installing your Spectrum Two FT-IR spectrometer, and follow the procedures described in this manual. If you require further assistance, go to www.perkinelmer.com/SpectrumTwoSupport.

Opening the shipping container

Your spectrometer is packed inside the shipping container, sealed inside a silver bag that protects the windows from condensation.

1. Remove the items from the box, and check that all the following parts are present:

Part Number	Description	Quantity
L9004169	USB 2.0 Cable (2 m)	1
L9002298	Power supply	1
L1202057	Polystyrene calibration film	1
L1600232	Spectrum Two J-stop card kit containing: 0.5 cm ⁻¹ , 1 cm ⁻¹ , 2 cm ⁻¹ , and 4 cm ⁻¹ J-stop cards and a half-aperture card	1
LX108873 OR LX108941 OR LX108875	Spectrum Standard Software (DVD) Spectrum Standard Software (USB Flash Drive) Spectrum ES Software (DVD)	1
L1050280	Spectrum Two Installation Video CD	1
L1050229	Spectrum Two Installation Guide (USB connection)	1
L1050242	Spectrum Two Manuals CD	1
L1250462	AVI calibration methane cell (Spectrum Two APV/AVI instruments only)	1

If any items are missing or damaged, go to www.perkinelmer.com/SpectrumTwoSupport for assistance.

2. Carefully remove the instrument from the shipping container, but not from the bag in which it was shipped.

Retain the original packaging in case you need to ship the instrument to a new location.

CAUTION

The spectrometer should be allowed to reach the temperature of its surroundings before it is removed from the protective bag to prevent condensation forming on the KBr windows (if applicable). This means leaving it for at least 3 hours after removal from the shipping container.

3. When the spectrometer has been allowed to warm to the temperature of its surroundings, remove it from the bag and place it on the bench where it is to be used. Ensure that you can reach the rear of the spectrometer to enable you to connect the cables.

NOTE: Do not connect your instrument to the PC using the USB cable provided until you have run the software installation wizard.

Any accessories will be shipped in separate boxes.

Choosing Your Connection Method

NOTE: Do not connect your instrument to the PC using the USB cable provided until you have run the software installation wizard.

The Spectrum Two spectrometer is supplied with a USB 2.0 cable and a mains power supply adaptor with a DC connector (Figure 9). The mains power cord supplied will depend on your region.



Figure 9 Connection cables supplied with the Spectrum Two

There are four ways you can connect to your spectrometer:

- Using the supplied USB 2.0 cable to connect directly to the PC.
This is the preferred method for direct connection to the spectrometer. The instrument will be configured automatically when you start Spectrum software.
- Using an Ethernet cable (not supplied) to connect directly to the PC.
If you want to connect your instrument directly to the PC using the Ethernet port, refer to the Administrator's Guide for your software for information on configuring the PC network adaptor. We recommend that you do this *before* installing Spectrum, Spectrum ES, or AssureID software.
- Over a wireless network using the PerkinElmer-configured wireless router (part number L1600246, not supplied with the spectrometer).
The optional wireless router enables you to locate your spectrometer away from the PC. This facilitates use of the spectrometer inside a fume cabinet or in a manufacturing environment.
Once you are connected to the instrument using the PerkinElmer FT-IR Wireless network, the instrument will automatically be configured on starting Spectrum software.
- Over a network using the Ethernet port.
If you want to connect your instrument over a network using the Ethernet port, refer to the Administrator's Guide for your software for information on configuring the IP address of your instrument, and details of the Instrument Install Wizard.

The features on the rear of the spectrometer are shown in Figure 10.

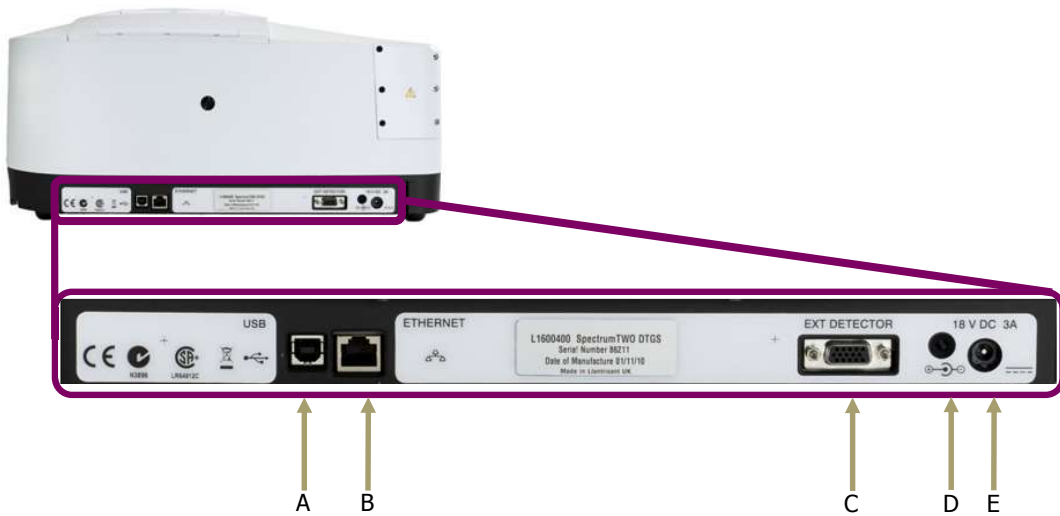




Figure 10 Communication ports on the Spectrum Two

Table 1 Communication ports

	Port/LED	Use
A	USB port 	This is the standard interface between the PC and the instrument.
B	ETHERNET port 	Ethernet connector. This is the standard interface between a Local Area Network (LAN) and the instrument.
C	EXT DETECTOR port	This port enables to you power the optional wireless router, accessory alignment tool, or connect an external accessory.
D	Rear diagnostic LED	Provides information on the status of the instrument. Refer to Table 2 on page 36.
E	DC power port	The DC power port is used to connect the spectrometer to the power supply. You can use the mains power supply adaptor and cable supplied, or you can use the optional battery pack or car adaptor.

NOTE: For more details of the port connector types, refer to *Appendix 1: Connector Details* on page 116.

Installing your Spectrum Two

NOTE: Do not connect your instrument to the PC using the USB cable provided until you have run the software installation wizard.

NOTE: If you wish to connect to your instrument using an Ethernet cable, you will need to configure the PC network adaptor. We recommend that you do this before installing your software.

- To install your software package (Spectrum, Spectrum ES, or AssureID, as required), insert the supplied DVD or USB Flash Drive and follow the instructions on the screen. You will need to select **Spectrum Two** as the Installation Type in Spectrum and Spectrum ES software.
If required, full installation instructions are provided in the Administrator's Guide for your software, which can be found on the *Spectrum Two Manuals CD* supplied with your instrument.
If you are supplying your own computer, make sure that it meets the minimum requirements for hardware and software set out in the "PC Requirements" section of the Administrator's Guide.

Spectrum and Spectrum ES software applications are available in German, English, Spanish, French, Italian, Japanese, Brazilian Portuguese and Simplified Chinese. The software language displayed is determined by the Region and Language settings defined for the operating system on the PC.

During the Spectrum software installation you will be provided with USB and wireless connection instructions (Figure 11). Connect your instrument to the mains power, and then set up your USB or wireless connection. For other connection methods, you do not need to connect up your instrument at this point. Refer to *Connecting the spectrometer to the PC using the USB cable* on page 36 or *Connecting the spectrometer to the PC using the wireless router* on page 38, as applicable.

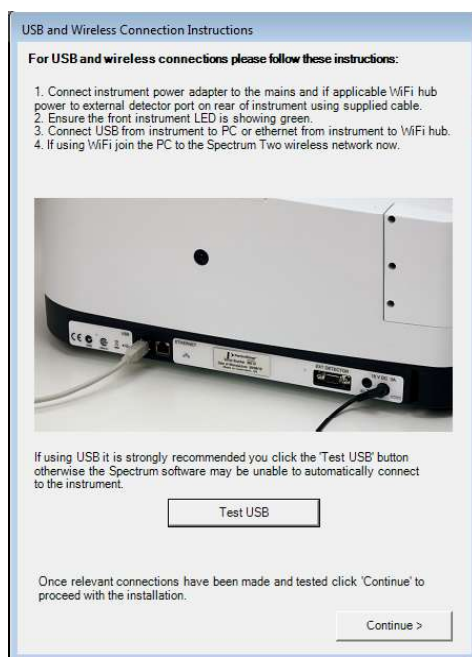


Figure 11 USB and Wireless Connection Instructions dialog

Connecting the spectrometer to the electrical supply

The Spectrum Two power supply adaptor can operate on electricity supplies of 50 or 60 Hz and in the 100 to 230 V range without any adjustment. The mains power cord supplied will depend on the requirements of your region.

NOTE: If it is necessary to fit a different plug on the power cord to the one supplied, refer to *Electrical safety* starting on page 14.

1. Ensure that your instrument is located near an appropriate mains power outlet.
2. Connect the cable from the power supply adaptor to the 18 V DC port on the rear of the instrument (Figure 12).



Figure 12 Power adaptor port on rear of the instrument

3. Connect the region-specific mains power cable provided to the power supply adaptor, and connect it to the mains power supply.
4. Switch on the power at the mains supply.
The instrument will power up automatically. The Power ON LED on the front of the instrument will be lit green (Figure 13).



Figure 13 Power ON LED

Your instrument will initialize and will then be ready to communicate with the PC. This will take approximately 2 minutes. During the initialization procedure the diagnostic LED on the rear of the instrument appears yellow as the instrument runs a series of self-checks. At the end of the initialization period, the diagnostic LED will flash orange.

Table 2 LED status

LED	Appearance	Status
Power ON (front of instrument)	Green, solid	Instrument is on.
	Yellow, flashing	Instrument is in Power Save mode (software controlled).
	Yellow, solid	Instrument is in Power Save mode (not software controlled).
	Off	Instrument is off. Check that the instrument is connected to the mains power.
Diagnostic (rear of instrument)	Yellow, solid	Instrument is running self-checks on initialization.
	Orange, flashing	Instrument is connected to mains power and is initialized.
	Red, flashing	Instrument has failed self-checks on initialization. You will not be able to connect to the instrument in the software. Refer to www.perkinelmer.com/SpectrumTwoSupport for assistance.
	Off	Instrument is off. Check that the instrument is connected to the mains power.

Before connecting your spectrometer to the PC you must install Spectrum, Spectrum ES or AssureID software.

NOTE: Once your instrument has been set up in one software application it will be available for use by all PerkinElmer FT-IR software installed on the PC.

Connecting the spectrometer to the PC using the USB cable

Before connecting your spectrometer to the PC via the USB cable you must run the Spectrum or Spectrum ES software installation. This is so that the appropriate drivers for the USB port are installed.

For Spectrum and Spectrum ES software, only connect the USB cable when prompted by the software Installation Wizard.

If you are using AssureID as stand-alone software, and have not previously installed Spectrum with Spectrum Two Installation Type, you will need to install the drivers for the USB connection. Refer to the *AssureID Administrator's Guide* (part number L1050019) for more information.

The following procedure describes connection using the USB 2.0 cable supplied with your instrument for Spectrum or Spectrum ES software:

1. When prompted by the Spectrum software installer, plug one end of the USB 2.0 cable provided into the USB port on the rear of the instrument (Figure 14).

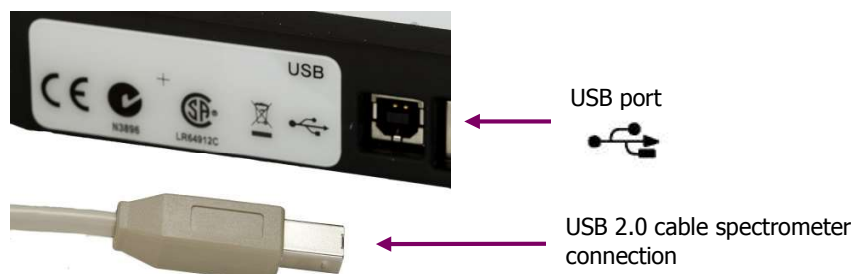


Figure 14 USB 2.0 cable connector and USB port

2. Plug the other end of the cable into a USB 2.0 port on your PC.
3. Click **Test USB** on the USB and Wireless Connection Instructions dialog. The software checks that the USB drivers have installed correctly and the result is displayed (Figure 15).

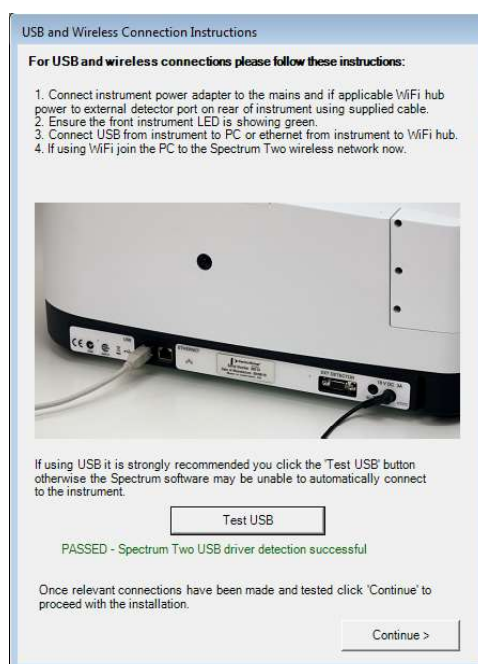


Figure 15 USB Wireless Connection Instructions – successful

If the test fails, check that the instrument is connected to the mains power and is connected to the PC using the USB 2.0 cable provided, and then retry the test.

If the test still fails, go to www.perkinelmer.com/SpectrumTwoSupport for assistance.

4. **Continue** the Spectrum software installation, following the instructions displayed on-screen.

You are now ready to start Spectrum software. The first time you log on to Spectrum with a Spectrum Two instrument connected to the PC via a USB cable, the instrument is installed and configured automatically.

NOTE: For AssureID, install the USB drivers, connect your spectrometer as shown in Figure 14, start AssureID, and then run the Instrument Install Wizard (see page 44). Refer to the *AssureID Administrator's Guide* (part number L1050019) for more information.

Connecting the spectrometer to the PC using the wireless router

The following procedure describes connection using the PerkinElmer-configured wireless router (not supplied with the instrument). The wireless router is powered by the EXT DETECTOR port on the rear of the Spectrum Two instrument. The cable required is supplied with the wireless router.

NOTE: If you are powering your instrument using the optional Spectrum Two Battery Pack (part number L1600233), powering the wireless router will reduce the runtime of the battery.

1. Unpack your wireless router, and position it near the instrument.
2. Connect the wireless router to the EXT DETECTOR port at the rear of the spectrometer using the cable supplied (part number L1602706), as shown in Figure 16.



Figure 16 Wireless router connected to the EXT DETECTOR port

3. Connect one end of the Ethernet cable to the ETHERNET port on the rear of the spectrometer and the other end to one of the ports numbered 1 to 4 on the rear of the router (Figure 17).

Do not use the blue port labeled INTERNET on the wireless router.



Figure 17 Ethernet cable connected to Port 4 on the wireless router and the Spectrum Two

4. Connect the cable from the power supply adaptor to the 18 V DC port on the rear of the instrument (Figure 18).



Figure 18 Power adaptor port on rear of spectrometer

5. Connect the Spectrum Two power supply cable to the mains power.
6. Ensure that the Power ON LED on the front of the Spectrum Two is lit green.
For more information on powering up your spectrometer, refer to *Connecting the spectrometer to the electrical supply* on page 35.

7. Ensure that the POWER LED on the front of the wireless router is lit green (Figure 19). The DIAG LED will be lit red while the router initializes.



Figure 19 POWER LED on the wireless router

8. Wait for the DIAG LED on the router to go out and ensure that the WIRELESS LED is lit (Figure 20).

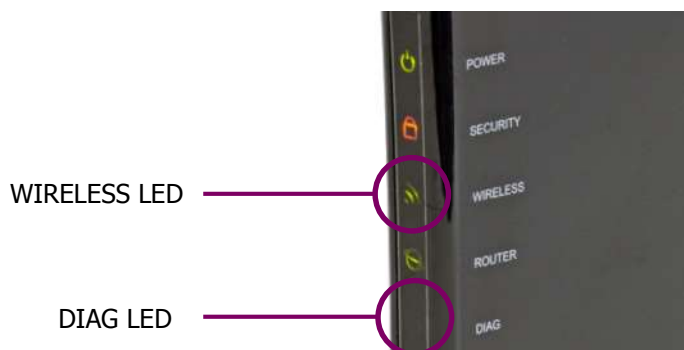


Figure 20 Wireless router LEDs indicate ready for use

9. Switch on your PC and then connect to the **PerkinElmer FT-IR Wireless** network. You will need to enter the network security key provided on the side of your router.



Figure 21 Connecting to the PerkinElmer FT-IR Wireless network (example only)

The exact procedure for connecting your PC to the wireless network will depend on your wireless hardware and on the PC operating system.

You are now ready to start your software application. The first time you log on to Spectrum with a Spectrum Two instrument connected to the PC via a wireless connection, the instrument is installed and configured automatically for you.

NOTE: For AssureID, connect your spectrometer as described in steps 1–9, start AssureID, and then run the Instrument Install Wizard (see page 44). Refer to the *AssureID Administrator's Guide* (part number L1050019) for more information.

NOTE: Although you can have more than one instrument on the wireless network, providing that each instrument has a unique IP address, you can only connect to one spectrometer at a time. PerkinElmer FT-IR software does not support simultaneous connection to multiple instruments on the same PC.

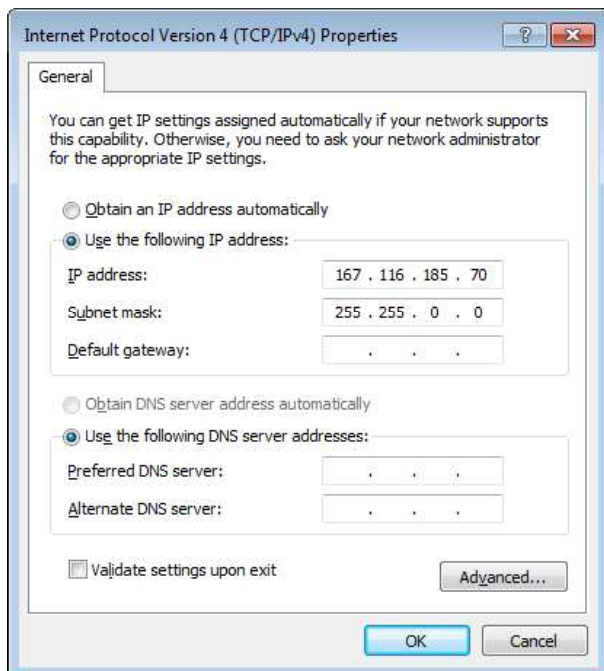
Connecting the spectrometer to the PC using an Ethernet cable

If you want to connect directly to your spectrometer via an Ethernet cable (not supplied), you must:

1. Configure the PC network adaptor to communicate with your spectrometer.

To connect to your instrument using an Ethernet port you will need to set up the TCP/IP protocols on the PC to be compatible with the spectrometer. You must do this *before* you start your software with your instrument connected to the PC.

If your PC is not on a network, you should type **167 . 116 . 185 . 70** as the IP address and type **255 . 255 . 0 . 0** as the subnet mask.



Refer to the Administrator's Guide for your software for a full procedure.

2. Plug one end of an Ethernet cable into the ETHERNET port on the rear of the instrument (Figure 22).

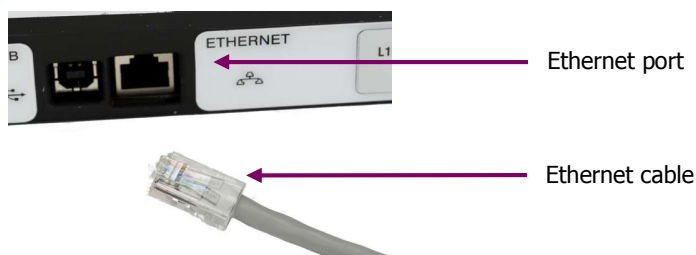


Figure 22 Ethernet cable connected to the ETHERNET port

3. Plug the other end of the cable into an Ethernet port on your PC.

You are now ready to start Spectrum software. The first time you log on to Spectrum with a Spectrum Two instrument connected to the PC using an Ethernet cable, the instrument is installed and configured automatically for you.

NOTE: For AssureID, configure the PC network adaptor, connect your spectrometer as shown in Figure 22, start AssureID, and then run the Instrument Install Wizard (see page 44). Refer to the *AssureID Administrator's Guide* (part number L1050019) for more information.

Connecting the spectrometer via a network

If you want to install your spectrometer using an Ethernet connection over a network you must:

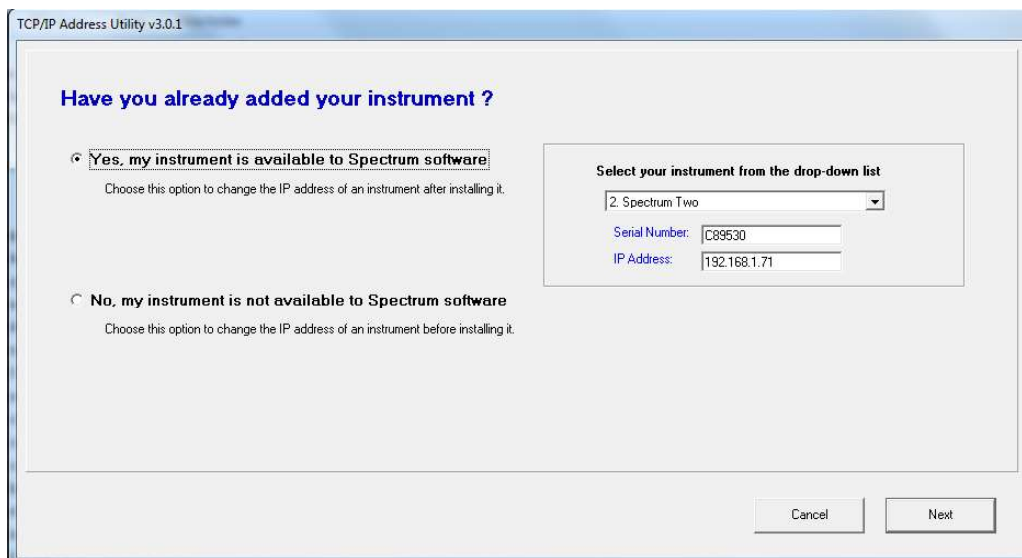
1. Assign the instrument a unique IP address that is compatible with your network using the Set IP Address Utility.

To run the utility, double-click **Set IP Address**, which is found in C:\Program Files\PerkinElmer\ServiceIR or C:\Program Files (x86)\PerkinElmer\ServiceIR.

NOTE: The TCP/IP address of the PC must be compatible with the instrument's IP address so that you can connect to the instrument using the Set IP Address utility. Refer to *Connecting the spectrometer to the PC using an Ethernet cable* above.

Select your instrument from the drop-down list. The default IP address of the instrument is **167 . 116 . 185 . 71**.

You can then assign a new IP address for the instrument.



When using a network, the TCP/IP port of the PC will normally obtain an automatic address from a DHCP server. To communicate with the instrument over a network, the instrument must have a compatible network address.

A subnet mask of **255 . 255 . 0 . 0** means that the first two parts of the instrument IP address must match the network IP address given to the PC by the DHCP server.

If, for example, the IP address of your PC is **195 . 112 . 170 . 255** and the subnet mask is **255 . 255 . 0 . 0**, then your instrument IP address must be **195 . 112 . x . x**.

Refer to the Administrator's Guide for your software for a full procedure.

2. Plug one end of an Ethernet cable into the ETHERNET port on the rear of the instrument (Figure 23).

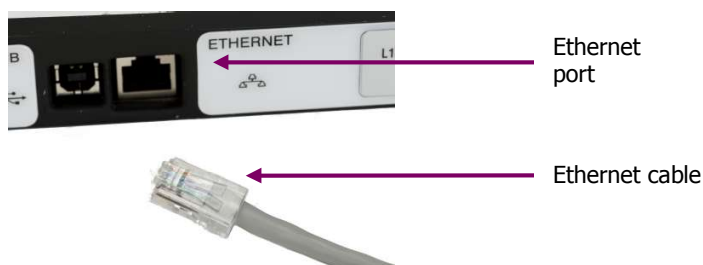


Figure 23 Ethernet cable connected to the ETHERNET port

3. Connect the other end of the Ethernet cable to the network router.
4. Add the instrument to the software using the Instrument Install Wizard, entering the IP address of the instrument when prompted.

Instrument Install Wizard

If you connected your spectrometer to a network using the Ethernet connection, or if you are using AssureID software to connect to the spectrometer, you will need to run the Instrument Install Wizard.

- If you have AssureID software, select **Configure Instruments** from the **Configure Instruments and Accessories** group on the Tools menu.
The Instrument Install Wizard starts.

OR

If you have Spectrum or Spectrum ES software, select **Add Instrument** from the **Instruments** group on the Setup menu.

The Instrument Install Wizard starts.

Details of the Instrument Install Wizard can be found in the Administrator's Guide for your software, which can be found on the *Spectrum Two Manuals CD*.

Changing the Sampling Accessory

NOTE: For full installation and usage instructions for your accessory, refer to the appropriate User's Guide available as a pdf on the *Spectrum Two Manuals CD* (part number L1050242).

1. If you are installing a UATR, you will need to remove the sample compartment cover (Figure 24), if fitted.
Open the cover, raise it to the vertical position and then lift it upwards, clear of the instrument.
Store the cover in a safe place for future re-use.



Figure 24 Removing the sample compartment cover

2. Remove the current sampling accessory by pulling the baseplate of the accessory towards you (Figure 25).



Figure 25 Removing the sampling accessory

3. If you are installing a UATR, pivot the accessory on the ledge at the front of the sample area (Figure 26a), and then tip it backwards (Figure 26b). Push it firmly, ensuring that the top of the accessory connects properly with the lid of the instrument.

If the accessory is pivoted too far forward on the sample area ledge it will not move correctly into position.

NOTE: Ensure that the transit block that secures the UATR pressure arm during transport has been removed. You may also need to remove the covers on the left and right sides of the accessory, and the top plate dust cover.



Figure 26 Installing the UATR accessory

OR

For other baseplate-mounted accessories, drop the accessory baseplate gently onto the ledge (Figure 27) and then slide it horizontally into the sample compartment.

Push the accessory firmly to ensure that the connector on the rear of the baseplate engages properly with the spectrometer connector.

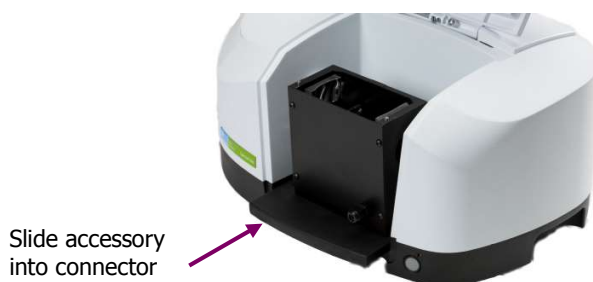


Figure 27 Installing the sampling accessory

Spectrum automatically recognizes which accessory is installed, and displays the accessory information on the Setup Instrument tabs.

The screenshot displays the 'Setup Instrument Basic' tab with the following settings:

- Actions:** Restore Defaults, Load and Save...
- Settings:**
 - Abcissa Units: Wavenumber
 - Start (cm-1): 4000
 - Ordinate Units: %T
 - End (cm-1): 515
- Scan Settings:**
 - Resolution (cm-1): 4
 - Scan Type: Sample
 - Data Interval (cm-1)
 - Accumulations: 4 Scans
- Accessory:**

Universal ATR	
Item	Value
Crystals	Diamond
Bounces	1
Serial Number	
UATR Options	Not Specified

Figure 28 Setup Instrument Basic tab showing a UATR

For information on using your accessory, refer to the User's Guide supplied with your accessory. For PerkinElmer Spectrum Two accessories, these can be found as pdf files on the *Spectrum Two Manuals CD* (part number L1050242).

Moving the Spectrometer



WARNING

Before moving the spectrometer, switch off the power supply, and disconnect the power cable.

The spectrometer can be lifted using the shaped handholds on its sides, as shown in Figure 29.



Figure 29 Lifting the Spectrum Two

For transportation between a car or laboratory, or between laboratories within your establishment, we recommend that you use the Spectrum Two Carry Case (part number L9004199).

If you need to ship your spectrometer, or return it to PerkinElmer following instrument replacement, you should use the original packaging.

NOTE: Refer to *Appendix 3: Decontamination and Cleaning* on page 118 for more information.

When moving your spectrometer between environments, be aware that the KBr sample compartment windows fitted in some Spectrum Two FT-IR spectrometers, although coated to prevent damage by small amounts of condensation, may be damaged by large amounts of condensation build-up in the rim of the windows.

Although the Spectrum Two spectrometer is usable within 15 minutes of being switched on after being switched off overnight, if your instrument has recently been transferred from a much colder environment it is advisable to run a background spectrum before every sample for the first couple of hours of use.

Getting Started with
Spectrum Software

Overview

This section describes some of the basic functionality available in Spectrum software. It will guide you through the process, from when you start Spectrum software to when you export your data, directing you to additional information where applicable.

It will show you how you can:

- Log in to Spectrum software
- Familiarize yourself with the Spectrum customizable workspace and the additional user assistance that is available: on-screen Help and Tutorials
- Check that the components of your spectrometer are working
- Collect a simple sample measurement
- Check/improve the quality of your spectrum
- Process your data in Spectrum software
- Extract your data from Spectrum software
- Change some advanced instrument settings
- Save energy with the Power Save mode
- Determine if your system is working as expected
- Exit Spectrum software, retaining your current work if required.


Starting Spectrum Software

1. Ensure that the instrument is connected to the mains power.
The Power LED on the front of the instrument should be lit green. If it is yellow, and you wish to connect to the instrument straight away hold down the power button on the front of the spectrometer for two seconds until the LED is lit green.
The instrument will initialize, which will take approximately 2 minutes.

NOTE: The Spectrum Two spectrometer is usable within 15 minutes of being switched on after being switched off overnight. However, if your instrument has recently been transferred from a much colder environment, it is advisable to run a background spectrum before every sample for the first couple of hours of use.

2. From the Start menu select **Programs**; the **PerkinElmer Applications** group; the **Spectrum** sub-group and then the **Spectrum** application.

OR


Double-click the shortcut icon  on the desktop.

The Spectrum start-up splash-screen is displayed, followed by a dialog that may require your login details:



The image shows a 'PerkinElmer Login' dialog box. It has a title bar with the text 'PerkinElmer Login'. Below the title bar, there is a key icon and the text 'Enter your user name and password.'. There are two text input fields: 'User name' and 'Password'. Below the 'Password' field is a 'Change Password...' button. At the bottom of the dialog are 'OK' and 'Cancel' buttons.

3. If required, enter your **User name** and **Password**, and then click **OK**.
The default user name and password are Administrator and administrator, respectively.
If you already have an instrument set up in Spectrum or AssureID software for this user on this PC, the Instrument Connection dialog may be displayed, unless Auto-Connect is set up for the instrument. If Auto-Connect is enabled, Spectrum will automatically connect to the instrument.



The image shows an 'Instrument Connection' dialog box. It has a title bar with the text 'Instrument Connection'. Below the title bar, there is the text 'Select an instrument to work with and press "Connect"'. There is a dropdown menu labeled 'Instrument:' with 'PerkinElmer FT-IR C86199' selected. To the right of the dropdown are 'Connect', 'Cancel', and 'Help' buttons. Below the dropdown is the text 'or click here to [work offline](#)'. There is a checked checkbox labeled 'Always connect to this Instrument'. At the bottom of the dialog, there is a 'Connection Status:' label and the text 'Currently Offline'.

NOTE: We recommend that you create a new user and password the first time you log on to Spectrum.

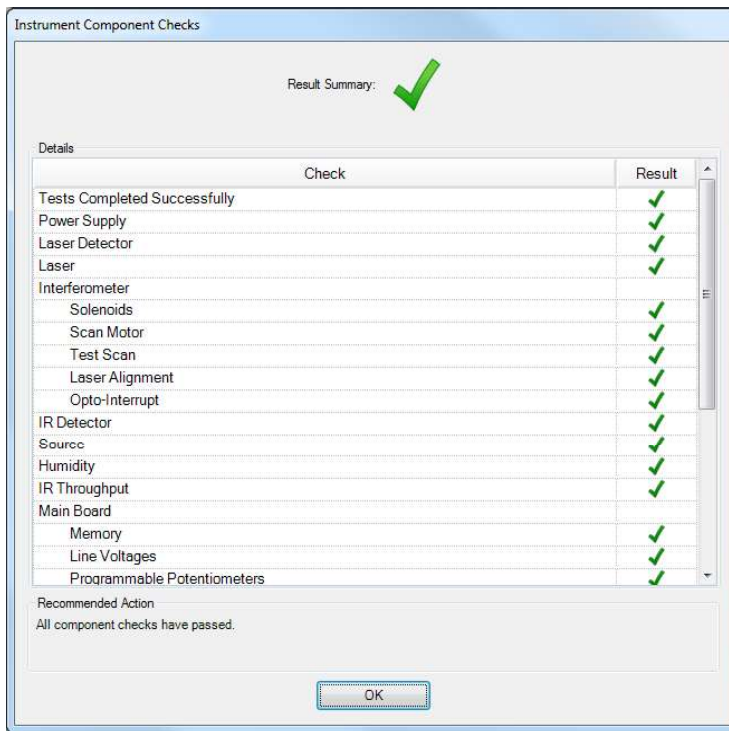
4. Select the **Instrument** you want to use and then click **Connect**.

OR

If you want to work with data that has been collected previously, without connecting to an instrument, select **work offline**.

Spectrum starts.

The first time you connect to your instrument the Component Checks will run.



5. When the Component Checks are complete, if there are no errors click **OK**.
You are now ready to collect data.
If a problem is identified, refer to *Component Checks* on page 81 for more information.

The Spectrum Workspace

The Spectrum window, with the default layout for a Spectrum Two installation, is shown in Figure 30.

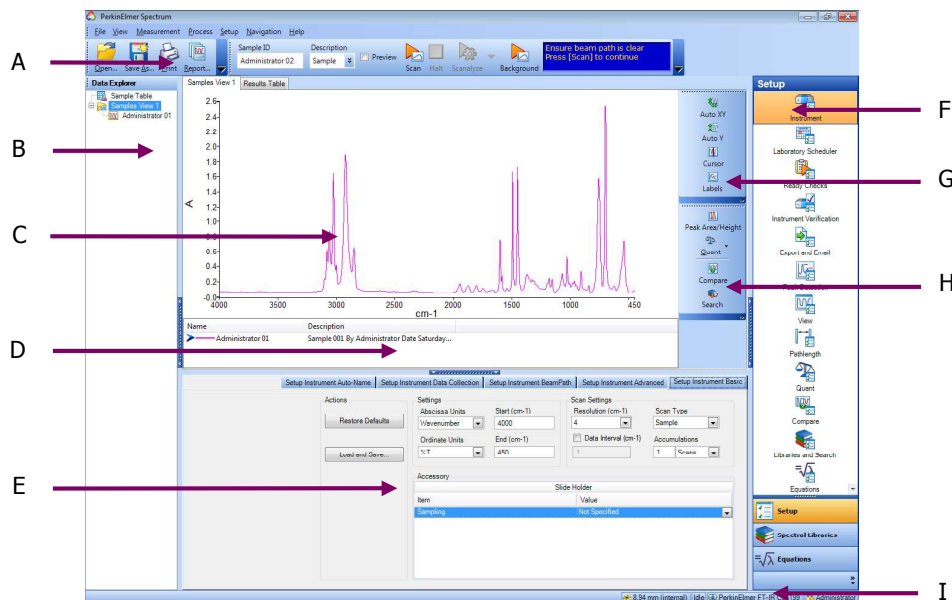



Figure 30 Spectrum window

A	Global Toolbars	F	Navigation Pane
B	Data Explorer	G	Graph Bar
C	Viewing Area	H	Process Bar
D	Information Pane	I	Status Bar
E	Dialog Pane		

The window is divided into four panes:

- The Viewing Area (C), in the center, where spectra or results are displayed.
- The Data Explorer (B), on the left, which you use to manage your spectra.
- The Navigation Pane (F), on the right, which contains shortcuts.
- The Dialog Pane (E), at the bottom, which you use to adjust parameters or enter information when, for example, setting up your instrument.

To open or close a pane, click .

NOTE: You can also click and drag the edge of a pane to resize it.

Viewing Area

The Viewing Area (C) is a tabbed display. The tabs displayed depend on whether you have an individual spectrum displayed, or whether you have selected a folder of spectra, known as a Samples View, in the Data Explorer. Tabs may be added that show the results of some processes, such as Compare, Search and Quant.

During scanning, the Live tab – which shows the spectrum in real time – may be displayed.

Data Explorer

Data Explorer (B), on the left, which you use to manage your spectra.

The item(s) selected in the Data Explorer will be displayed in the Viewing Area.

You can also use the Data Explorer to access the Sample Table, which enables you to set up multiple samples for data collection.

Navigation Pane

The Navigation Pane (F), on the right, which contains shortcuts.

The Setup options are the same as the Setup menu items. The Equations and Spectral Libraries options on the Navigation Pane enable you to see a list of the available equations and libraries, respectively.

You can reorder the shortcuts in the Navigation pane so that those you use most often are easier to access. Simply drag-and-drop the shortcut to a new position.

Dialog Pane

The Dialog Pane (E), at the bottom, which you use to adjust parameters or enter information when, for example, setting up your instrument or a Compare processes.

The contents of the Dialog Pane reflect the shortcut selected in the Navigation Pane.

Global Toolbars

At the top of the workspace are the Global toolbars (A), which include the File bar and the Measurement bar (displayed by default), and the optional Instrument Settings bar.

NOTE: The Spectrum toolbars can be individually customized, and new toolbars can be added. For more information, refer to the Spectrum on-screen Help and the tutorial **Customizing Toolbars**. These can be accessed from the Help menu.

Graph Toolbars

If the Graph or Samples View tab is displayed, you can see the local Graph toolbars. The Graph bar (G) contains some tools that enable you to change how data is displayed in the graph, and the Process bar (H) enables you to access shortcuts to processes that enable you to manipulate your data.

NOTE: The Spectrum toolbars can be individually customized, and new toolbars can be added. For more information, refer to the Spectrum on-screen Help and the tutorial **Customizing Toolbars**. These can be accessed from the Help menu.

Information Pane

Below the graph in the viewing area is the Information Pane (D). This shows a curve selector if you have selected a Samples View in the Data Explorer or, if an individual spectrum is selected, shows the results for that spectrum.

Status Bar

The Status Bar (I) located at the bottom of the workspace shows user information, messages, and the current status of the instrument.

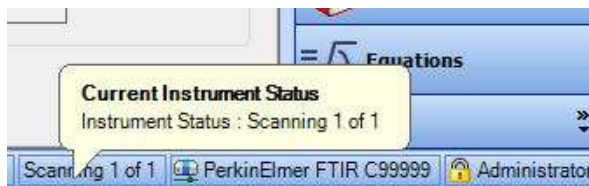


Figure 31 Status bar

Using the Spectrum on-screen Help system

Use the Spectrum Help system to find further information about using Spectrum software to control, set up and adjust your instrument.

To open the Help file, select **C**ontents from the Help menu. This menu also includes links to on-screen tutorials (**T**utorials), and information about the software (**A**bout).

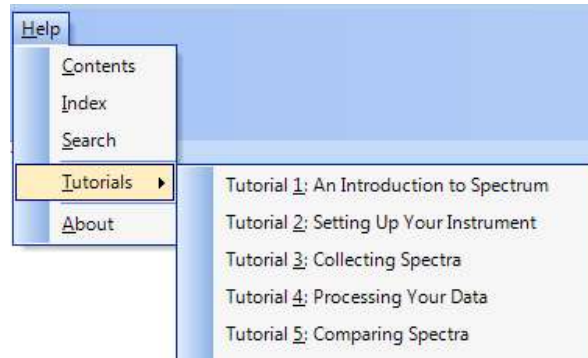


Figure 32 Help menu in Spectrum Software

Scanning Samples

When you connect to your Spectrum Two, the instrument settings will default to appropriate values for your instrument and accessory. These should be suitable for most applications. The default scan range is 4000 to 450 cm^{-1} .

The Measurement bar (Figure 33) displayed by default at the top of the workspace includes the tools you need to collect a spectrum from a sample. You can also select these commands from the Measurement menu.



Figure 33 Spectrum Two Measurement bar


1. If you want, enter a unique **Sample ID** and **Description** for the sample on the Instrument Settings toolbar.
Alternatively you can use the Autaname function to enter a unique Sample ID and Description for each scan. The default Sample ID is [User name]_nnn, but you can configure this on the Setup Instrument Data Collection tab. For more information, see the Spectrum on-screen help.
2. If a background scan is required, the **Scan** button includes a small background flag. Clear the instrument beam path, or insert a suitable background material, and then click




to collect a background spectrum.

If using an ATR Accessory, ensure that the crystal is clean before collecting a background.

The background spectrum is displayed briefly, and then the Viewing Area is prepared for data collection from your sample.

3. Place your sample in the instrument and then click  .
By default, during scanning the sample data is displayed on the Live tab in the Viewing Area.
The completed spectrum is displayed on the Graph tab (Figure 34), and added to the current Samples View in the Data Explorer. Your spectrum will be saved automatically. See *Auto-Save Spectra* on page 72 for more information.
The results of the Quality Checks, selected by default on the Setup Instrument Advanced tab, are displayed in the results for the spectrum. See *Quality Checks* on page 59 for more information.

NOTE: If Preview is selected on the Measurement toolbar; the spectrum will be displayed on the Live tab in the Viewing Area. This live spectrum will be automatically updated, but no data will be collected. This enables you to verify that your sample is suitable or, if using an ATR accessory, that there is good contact between the sample and the crystal. When you are happy with the spectrum, click  to begin collecting data.

If, for any reason, you want to stop scanning your sample, click  .

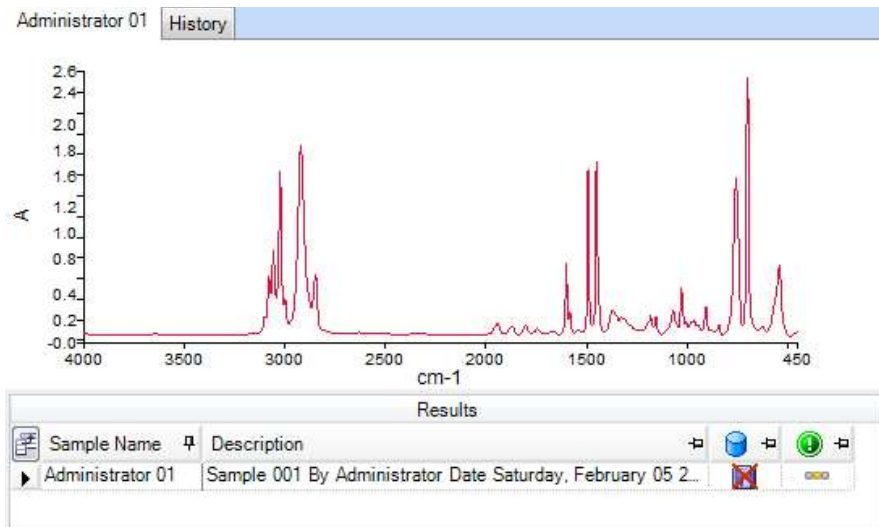


Figure 34 Spectrum displayed in the Viewing Area

If you want to change any of the default instrument settings, select **Instrument** from the Setup menu to display the Setup Instrument tabs. For more information see *Instrument Settings* on page 78.

Quality Checks

Quality Checks identify possible problems in the collected spectrum and suggest ways of improving the measurement.

Quality Checks can be selected on the Setup Instrument Advanced tab (Figure 35). Simply select the **Quality Checks** that you want to perform from the list in the Setup Instrument Advanced tab and, if required, adjust the threshold **Range** using the slider bars to suit your application.

To display more information about an individual test, double-click on its name in the list to display the Quality Checks Help.

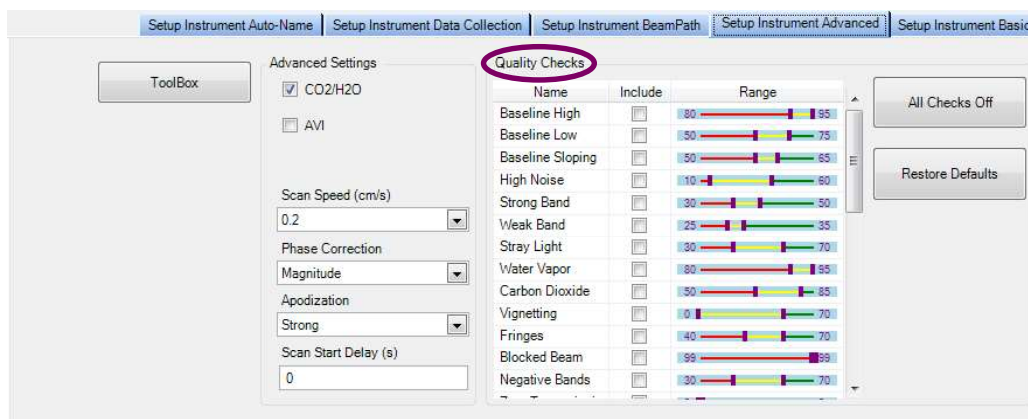








Figure 35 Setup Instrument Advanced tab in Spectrum

When you collect your spectrum, the selected tests are performed as the data is collected and a signal light (green , amber , or red ) indicates the result.

Signal	Result	Meaning
	Passed	The quality of the spectra is satisfactory.
	Caution	There is a problem that you may want to investigate to improve the quality of the spectra you are collecting.
	Warning	There is a serious problem that you should attempt to solve before collecting further spectra.

The result is displayed in the Results Table, and in the Information Pane for an individual spectrum. For example, the Quality Checks reported multiple warnings for the spectrum shown in Figure 36.

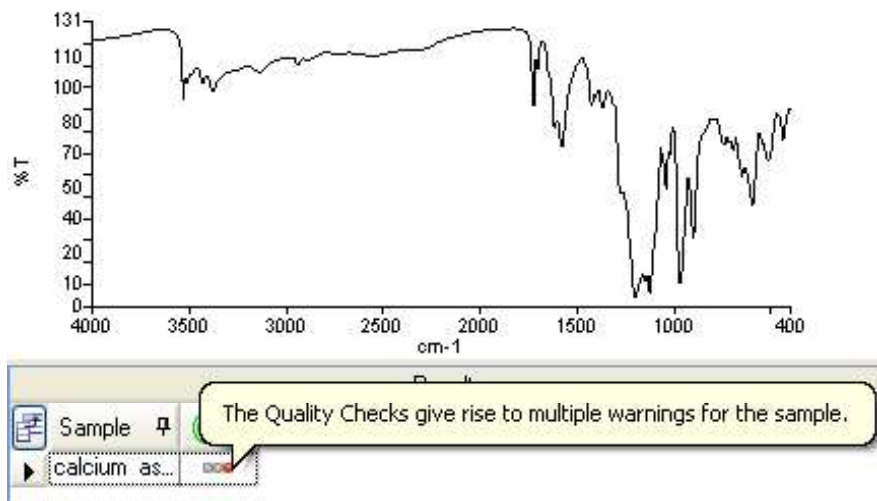


Figure 36 Quality Checks result shown in the Information Pane

To see which Quality Checks passed and which identified a problem, select the History tab of the spectrum in the Viewing Area and refer to the Quality Checks section of the tab (Figure 37).

Quality Checks	
Setting	Value
Water Vapor	Passed
Carbon Dioxide	Passed
Baseline Low	Passed
Baseline High	Warning
Baseline Slope	Passed
Strong Bands	Passed
Weak Bands	Passed
High Noise	Passed
Fringes	Warning
Vignetting	Passed
Blocked Beam	Passed
Negative Bands	Passed
Zero Transmission	Passed
Stray Light	Passed
Window Cutoff	Passed

Figure 37 History tab showing the results of the individual Quality Checks

For each check that failed, refer to the Quality Checks Help for suggestions on how to stop it occurring again.

Processing Spectra

To process your data in Spectrum software, ensure that the spectra you wish to process are selected in the Data Explorer and then select the appropriate option from the Process menu (Figure 38).

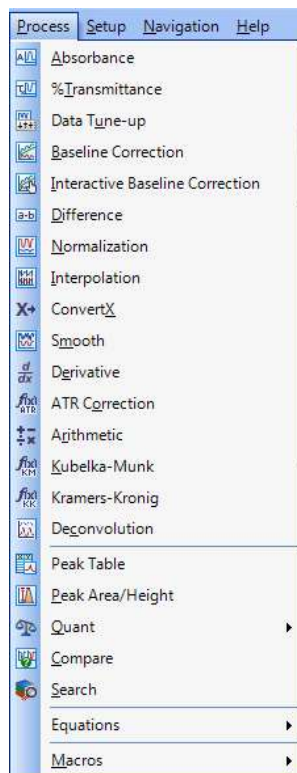


Figure 38 Process menu in Spectrum

When the spectra have been processed, if the process generated new spectra they will be added to the Data Explorer with `_n` appended to the name to create a unique Sample ID. Spectra created by processing are not saved automatically. For more information, see *Saving spectra* on page 72.

NOTE: For full details of each process, refer to the Spectrum on-screen Help.

Spectral correction

Several processes in Spectrum enable you to adjust your spectra after data collection. For example, there are commands for the conversions of ordinate units, such as: Absorbance, Transmittance, Kubelka–Munk and Convert X.

You can also correct for baseline slope in your spectra. In Spectrum you can do this in two ways: using an automatic baseline correction, or using an interactive baseline correction (i-baseline) that enables you to define base points for the conversion (Figure 39).

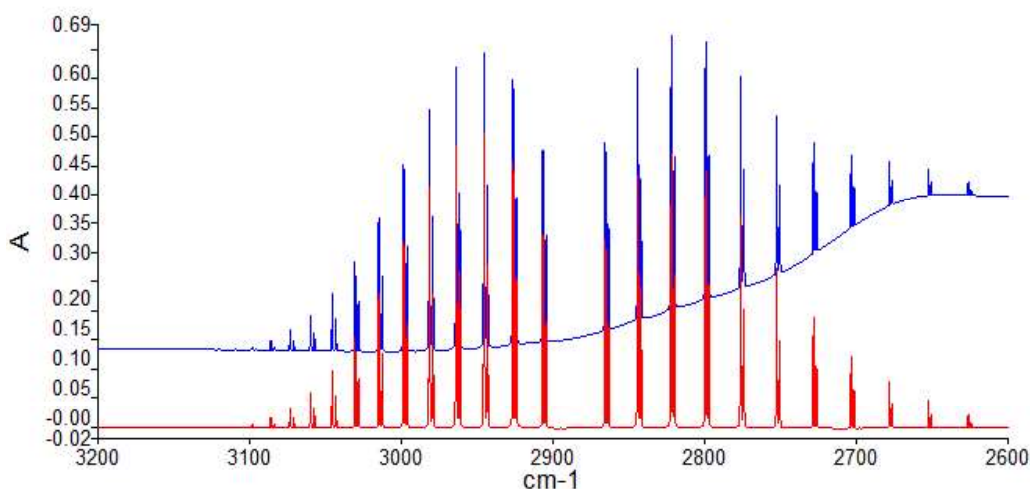


Figure 39 Spectrum with baseline corrected using i-baseline

NOTE: The **Processing Your Data** tutorial includes a description of ordinate-unit conversion, automatic baseline correction, and peak detection and labeling.

Identification

Several processes in Spectrum can be used to help identify your sample.

Peak Table

The results of a peak table can be used to compare peaks with another sample – for example, one published in a pharmacopoeia. The results of the process are displayed on the Peak Table tab in the Viewing Area (Figure 40).

Spectrum Name	Peak Name	X	Y
acetone-A	1	3414.28	84.14
	2	3004.68	74.54
	3	1715.85	6.35
	4	1421.07	62.77
	5	1363.03	26.03
	6	1222.37	23.67
	7	1092.54	78.47
	8	902.59	84.59
	9	530.24	58.83

Figure 40 Peak Table tab

- Select **Peak Detection** from the Setup menu to display the Setup Peak Detection tab and define the thresholds and the algorithm used to identify the peaks.

NOTE: You can also add peak labels to the spectrum using the same thresholds using the **Label Peaks** option on the View menu.

Compare

The Compare process estimates similarity between spectra by comparison with a reference spectrum or spectra, and is used to confirm the identity of a sample. The results are displayed on the Compare tab in the Viewing Area (Figure 41).

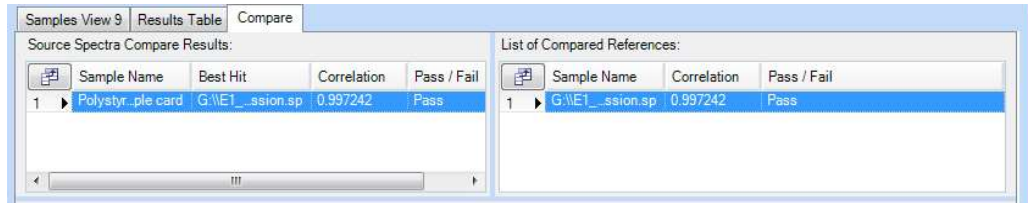


Figure 41 Compare tab

In this example, the spectrum has been confirmed to be the same as the reference spectrum, where the Correlation was defined at 0.98. The Correlation result is greater than 0.99, where 1.00 would mean that the spectra were identical.

NOTE: For an example of a Report generated showing the Compare results, refer to **Reporting** on page 76.

The parameters used in the Compare process are defined on the Setup Compare tabs.

- Select **Compare** from the Setup menu to display the Setup Compare tabs.

On the Setup Compare References tab (Figure 42) you can load a single spectrum file or a folder of spectra. Then set the Correlation and/or Discrimination thresholds to define the Pass/Fail result.

Correlation expresses the degree of similarity between the spectra, where 1 is identical, and 0 is wholly unrelated. Discrimination ensures that the closest match is sufficiently separated from the next closest match. Its value is the difference in the Correlation values of the first two results on the Compare tab.

Only files or folders with **Include** enabled will be used in the Compare.

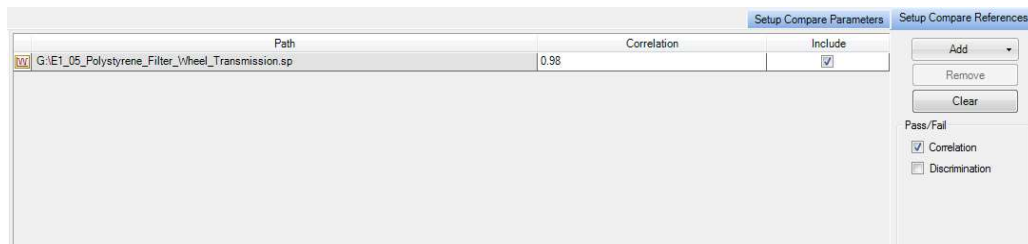


Figure 42 Setup Compare References tab

On the Setup Compare Parameters tab (Figure 43) you can define a limited wavelength range of your spectrum to be compared with the reference spectrum or spectra, and apply filters that try to eliminate differences in spectra that are not related to differences in the sample, such as differences between instruments or environmental condition. Refer to the Spectrum on-screen help for more information.

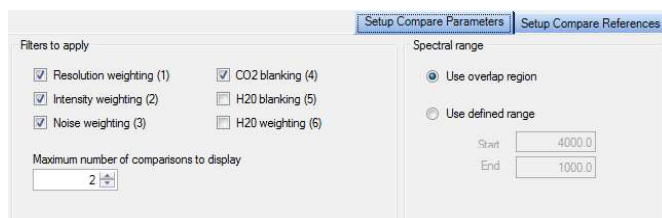


Figure 43 Setup Compare Parameters tab

NOTE: The **Comparing Spectra** tutorial worked example compares the results of a spectra subtraction (using the Difference process) to a reference spectrum.

Search

The Search process is used to confirm the identity of an unknown sample by comparison with a reference library or spectra. The results are displayed on the Search tab in the Viewing Area (Figure 44).

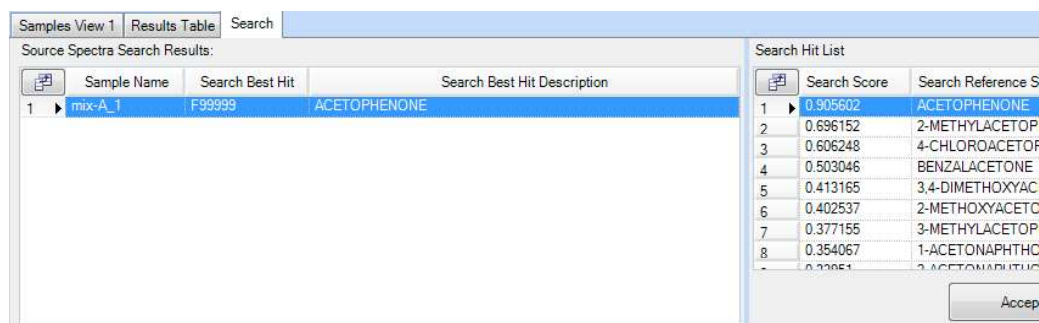


Figure 44 Search tab

In the upper left quadrant the name of your source spectrum or spectra are displayed, with the Search Best Hit. In this example the Best Hit was acetophenone. For each source spectrum selected, all the results are displayed in the Search Hit list. If you want to select an alternative Search Best Hit, you can click **Accept as best hit**.

The best hit spectra are displayed in a graph below the Source Spectra Search Results, in the lower left quadrant of the Search tab.

NOTE: You can also use the Search process for a Mixture Search. Refer to the Spectrum on-screen help for more information.

The parameters used in the Search process are defined on the Setup Libraries and Search tabs.

- Select **Search** from the Setup menu to display the Setup Libraries and Search tabs.

Select which folders or files are available as Spectral Libraries on the Setup Spectral Libraries tab (Figure 45), and specify which of the available spectral libraries should be included in the Search Process. Only files or folders with **Include** enabled will be used in the Search.

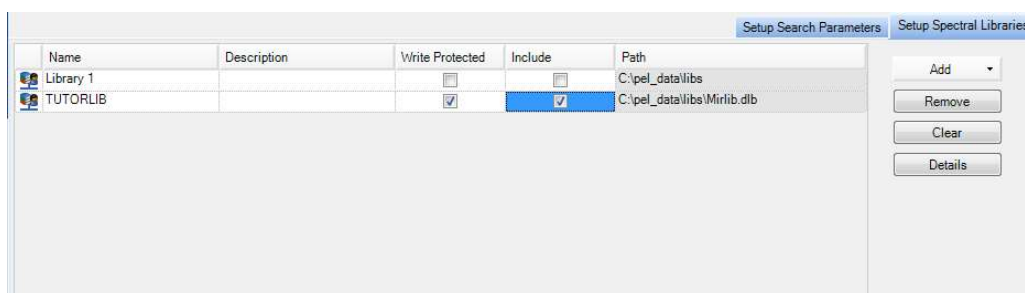


Figure 45 Setup Spectral Libraries tab

On the Setup Search Parameters tab (Figure 46), enter the maximum number of best hits to display in the Search tab when a Search process is run. By default your spectrum is compared with each reference spectrum over the range where the spectra overlap. But if you are particularly interested in a region select a **User defined range**, and/or if you want to exclude regions from the spectra, enter the appropriate **Start** and **End** values in the Blank Regions section.

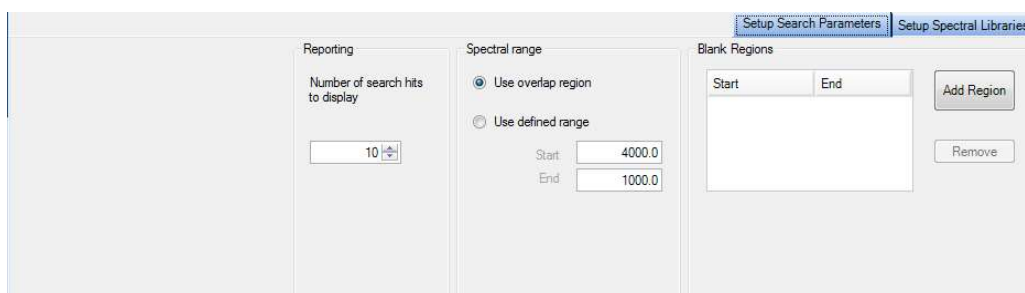


Figure 46 Setup Search Parameters tab

The Libraries available in Spectrum are listed in the **Spectral Libraries** section of the Navigation Pane. Double-click on the library icon to administer your library (for user-defined libraries you can add or remove spectra), or to view information about the library or spectra (Figure 47). For example, you can view any properties associated with a particular spectrum or the image of a structural unit.



Figure 47 Library details

NOTE: The **Search** tutorial provides an example of using the Search process to identify an unknown contaminant in a sample.

Quantification

Peak Area/Height

Use the Peak Area/Height process to produce a table of the peak areas and/or peak heights for your spectrum or spectra. You can process spectra individually, or select a spectrum on which to define the parameters that will be used for a number of spectra.

The height can be defined at a point (**Height**), or as the maximum height between two points (**Max Height**). The **Bases** section enables you to define the baseline that is used when determining the peak area or height.

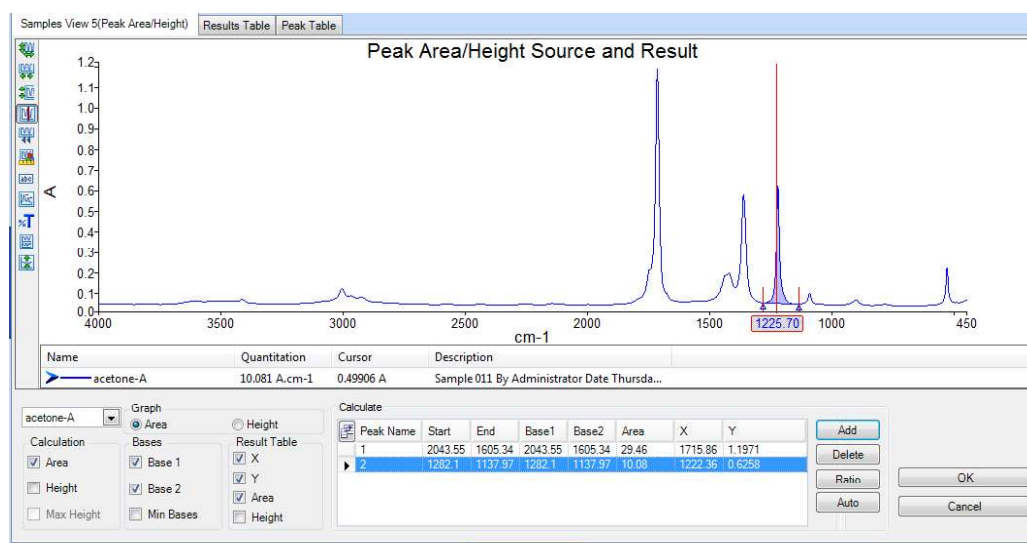


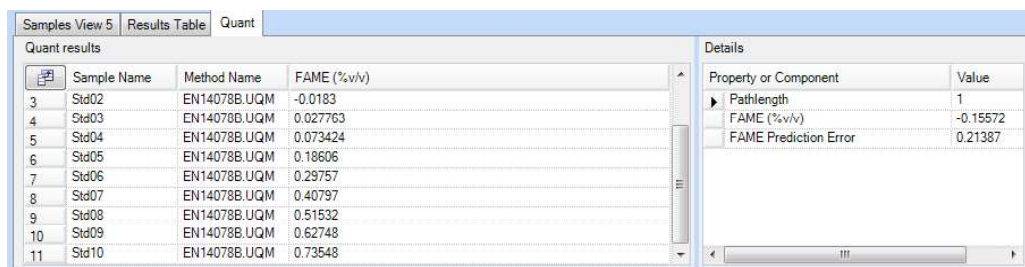
Figure 48 Peak Area/Height dialog

When the Peak Area/Height process is run, the results are shown on the Peak Table tab (Figure 40).

Quant

The Quant process is used to quantify properties of a sample by using one or more Quant methods created using the Spectrum Quant Builders. The Spectrum Quant Builder software enables you to build a method using a set of standard spectra that you have collected. Once the method has been built and then validated in the Quant Builder software, it can be used to quantify a component in your sample spectrum.

The results are displayed on the Quant tab in the Viewing Area (Figure 49), and in the Results table. In this example, the Prediction Property calculated by the Beer's Law algorithm was FAME (fatty acid methyl ester) concentration in % v/v.



Sample Name	Method Name	FAME (%v/v)
Std02	EN14078B.UQM	-0.0183
Std03	EN14078B.UQM	0.027763
Std04	EN14078B.UQM	0.073424
Std05	EN14078B.UQM	0.18606
Std06	EN14078B.UQM	0.29757
Std07	EN14078B.UQM	0.40797
Std08	EN14078B.UQM	0.51532
Std09	EN14078B.UQM	0.62748
Std10	EN14078B.UQM	0.73548

Property or Component	Value
Pathlength	1
FAME (%v/v)	-0.15572
FAME Prediction Error	0.21387

Figure 49 Quant tab

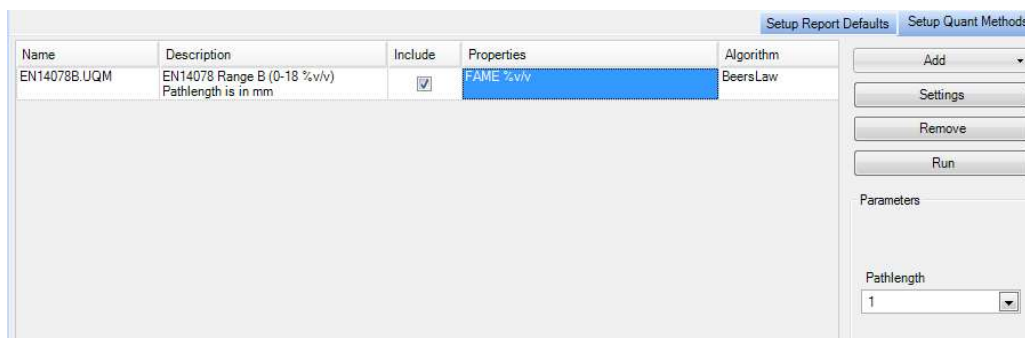
In the upper left quadrant your source spectrum or spectra are displayed, with the Quant prediction results. For each source spectrum selected, more information is shown in the Details section.

For each sample, the source spectrum and any spectra generated as part of the analysis are displayed in the graph below the Quant results, in the lower left quadrant of the Search tab.

The Quant methods used in the Quant prediction are defined on the Setup Quant Methods tab:

- Select **Quant** from the Setup menu to display the Setup Quant tabs.

Select which Quant methods are available on the Setup Quant Methods tab (Figure 50), and specify which of the available methods should be included in the Quant prediction. Only files or folders with **Include** enabled will be used to process the spectra.



Name	Description	Include	Properties	Algorithm
EN14078B.UQM	EN14078 Range B (0-18 %v/v) Pathlength is in mm	<input checked="" type="checkbox"/>	FAME %v/v	BeersLaw

Property or Component	Value
Pathlength	1

Figure 50 Setup Quant Methods tab

More information about the method selected is shown in the Quant Method Setup dialog (Figure 51):

- Select **Settings** on the Setup Quant Methods tab.
Here you can view a summary of the Quant method and, where the Quant calibration includes more than one prediction Property, select which ones will be included when the Quant method is run (Figure 51).

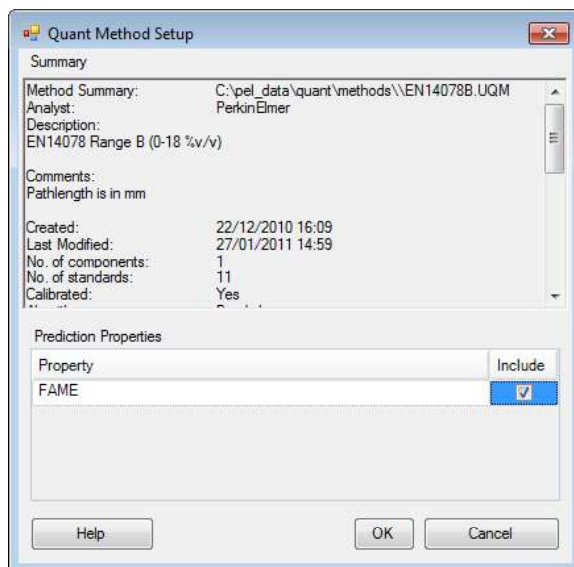


Figure 51 Quant method details

On the Setup Report Defaults tab (Figure 52), select which prediction results will be displayed for each algorithm type in the Results Table when a Quant prediction is run.

Algorithm	Value	Calculate value	Display value by default
QuantPlusPLS1	PropertyRMSError	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS1	PropertyP2PError	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS1	PropertyMDistance	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS1	PropertyResidualRatio	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS1	PropertyResidualSpectrum	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS1	PropertyCalculatedSpectrum	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS1	PropertyPredictionError	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPCR	MethodRMSError	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPCR	MethodP2PError	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPCR	MethodTotalMDistance	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPCR	MethodResidualRatio	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPCR	PropertyMDistance	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPCR	MethodResidualSpectrum	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPCR	MethodCalculatedSpectrum	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPCR	PropertyPredictionError	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS2	MethodRMSError	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS2	MethodP2PError	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS2	MethodTotalMDistance	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS2	MethodResidualRatio	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS2	PropertyMDistance	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS2	MethodResidualSpectrum	<input checked="" type="checkbox"/>	<input type="checkbox"/>
QuantPlusPLS2	MethodCalculatedSpectrum	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Figure 52 Setup Quant Results tab

NOTE: Refer to the Spectrum on-screen Help for more information.

Equations

A list of the available Equations is displayed on the Setup Equations tab. The Equations are also added to the Equations sub-menu of the Process menu.

- To add a new Equation, select **Equations** from the Setup menu to display the Setup Equations tab, and then select **Add**.
The Equation tab will be displayed (Figure 53).

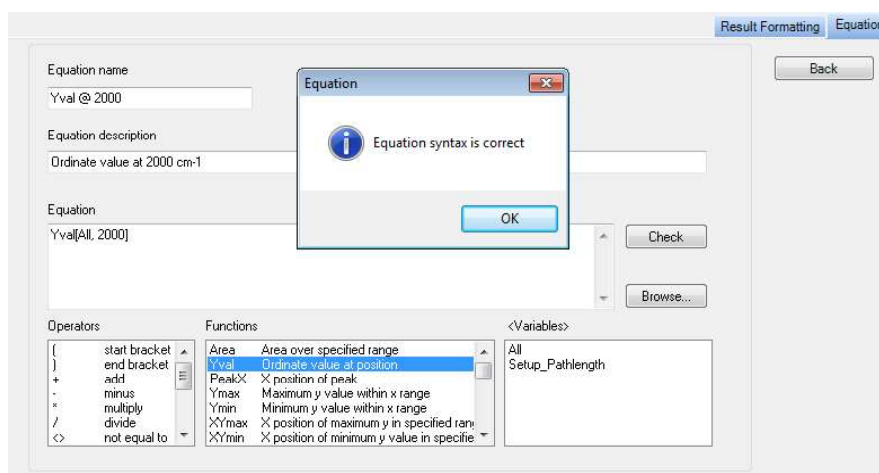


Figure 53 Equation tab

You can type in an equation, or click on items in the **Operators**, **Functions** or **Variables** lists. Each function has a number of required or optional arguments. A tooltip will be displayed when you enter a function to show you the correct syntax. The first argument is often **<spectrum>**, which if set to **All** will be applied to all spectra selected, but you can Browse to select a specific spectrum.

Any results in the Results table will be available as **Variables**, as well as the pathlength set on the Setup Pathlength tab. In this way you can add numeric custom columns in the Sample Table for your spectra and these entries will be available for use in equations.

When you have finished entering your equation, you can click **Check** to verify your equation.

NOTE: The **Macros** tutorial provides an example of using an Equation to calculate the area of a peak.

The Results formatting tab enables you to define Pass / Fail criteria and select how the result will be displayed. For example, you can color the cell in the Results Table green if the result is a Pass.

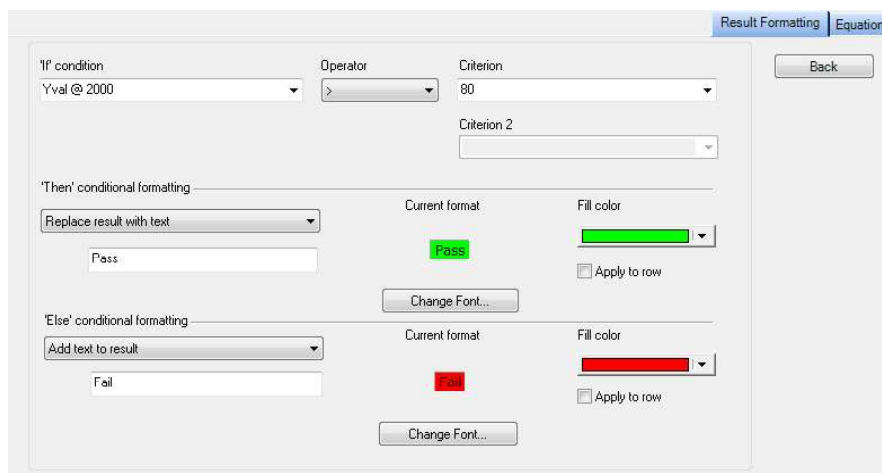


Figure 54 Results formatting example

To view the details of, or modify, an equation:

- Select **Equations** in the Navigation Pane and then select the appropriate icon.

OR

Select the Equation on the Setup Equations tab, and then click **Settings**.

To run the equation, select the spectrum or spectra you want to process in the Data Explorer, and then select the equation from the Equations sub-menu of the Process menu.

Macros

As well as performing the individual process commands you can combine these to create a workflow or Macro. Macros can also include Instrument Setup (Figure 55) and Data Collection, and export and reporting commands to enable you to structure your analysis from setting the instrument parameters to generating your results.

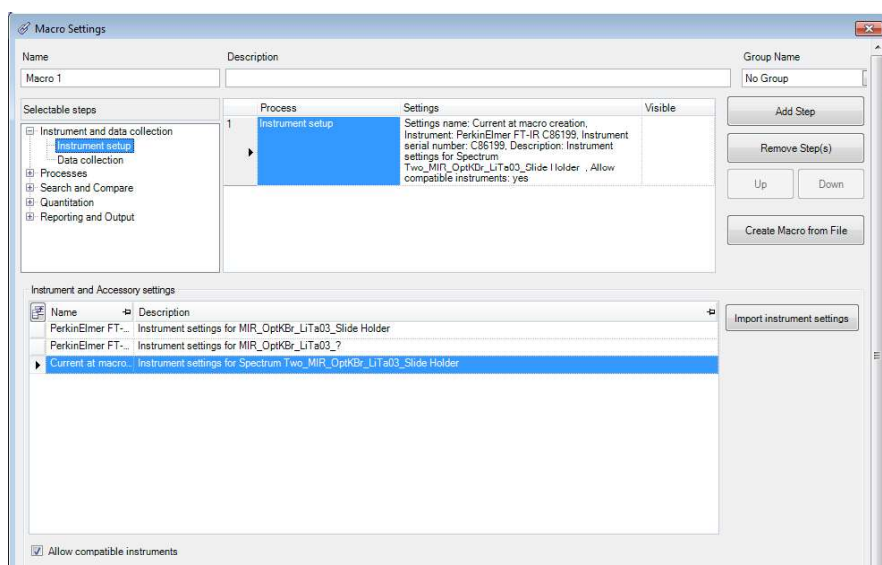


Figure 55 Macros Settings dialog showing an Instrument Setup step

NOTE: Refer to the **Macros** tutorial and the on-screen Help for more information.

Scanalyze

As well as Macros, you can use the Scanalyze feature in Spectrum to scan a spectrum and then immediately process it using the Compare, Quant or Search options. During multiple accumulations, the results are displayed and then updated as the data collection progresses.

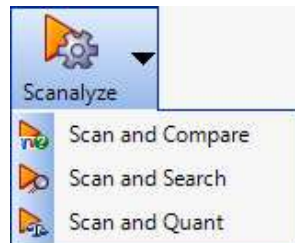


Figure 56 Scanalyze options

The Compare, Quant and Search processes must first be set up using the appropriate Setup menu option.

NOTE: You must have a valid background for the Scanalyze option to be available.

Saving Spectra, Exporting Spectra and Reporting

There are various features in the software to help you present your data outside Spectrum.

Saving spectra

All spectra in Spectrum software are saved to *.sp format by default.

To find out if a spectrum has been saved, refer to the Results Table (if a Samples View is selected) or the Information Pane. Spectra that are not saved are marked by a red cross.

In Figure 57 the original spectra have been saved to disk, but the processed spectrum, with _1 appended, has not.

Sample Name	Description	Best Hit	Pass / Fail
blistab	Paracetamol tabl...	✓	Pass
blister	Paracetamol blist...	✓	Pass
blistab_1	Paracetamol tablet	✗	Fail

Figure 57 Saved and unsaved spectra displayed in the Results Table

You can save your spectra in the following ways:

- Using the Auto-Save option when collecting spectra
- Using the Save, Save As and Save All options from the File menu
- Using an Output step in a Macro
- Using the context menu in the Viewing Area.

Auto-Save Spectra

In Spectrum software, Auto-Save is selected by default (Figure 58). This will save your spectra to the folder specified after each measurement.

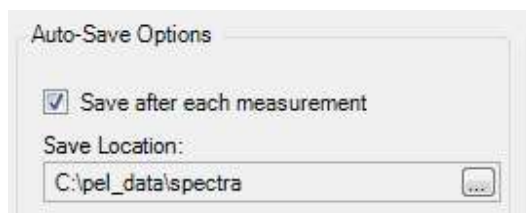


Figure 58 Auto-Save spectra on the Setup Instrument Data Collection tab

The default Save Location, here C:\pel_data\spectra, was defined during the software installation. If you wish to change the location, or deselect this option, refer to the Setup Instrument Data Collection tab.

Save, Save As, Save All

Save will save the selected spectrum, or the spectra in the selected Samples View, to the current default save location.

Save As displays a dialog for the spectra selected that enables you to change the file name and the destination directory (Figure 59). You can also change the default save location for all spectra.

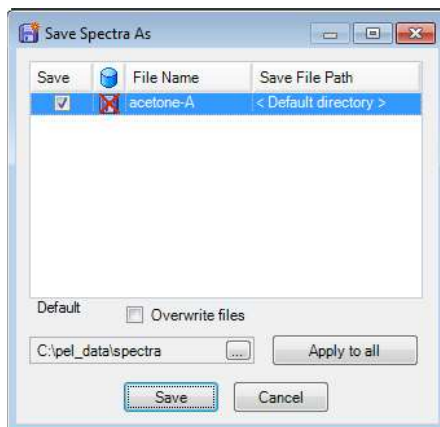


Figure 59 Save Spectra As dialog

Save All displays a dialog similar to that shown in Figure 59, but listing all the spectra open in Spectrum.

Save Binary

Use the Save Binary option in the graph to save the spectrum as a *.sp file. Select a curve and then right-click to display a context menu. Select **Save Binary**, and then browse to a save location.

Exporting spectra

You can export spectra in several ways:

- Using the Auto-Save Export option when generating spectra
- Using the Export option from the File menu
- Using an Output step in a Macro
- Using the context menu in the Viewing Area (ASCII format only).

You can export your spectra to csv format, JCAMP-dx, ASCII, or a custom format. The settings for the Custom Defined Format are selected on the Setup Export tab. Refer to the Spectrum on-screen Help for more information.

Auto-Save Export

If you select **Export** on the Setup Instrument Data Collection tab, your spectra will be exported to the location specified after each measurement (Figure 60).

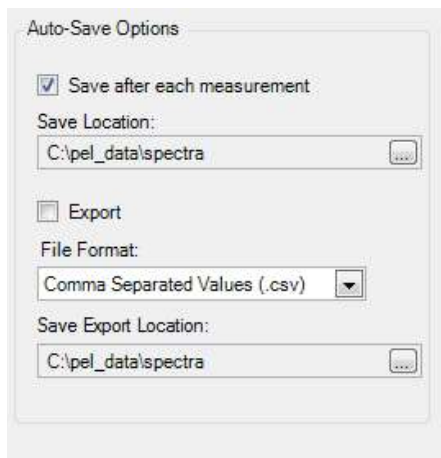


Figure 60 Auto-export on the Setup Instrument Data Collection tab

The default Save Location, here C:\pel_data\spectra, was defined during the software installation. To select this option, or to change the default save location, refer to the Setup Instrument Data Collection tab.

Export

You can export your spectra at any time using the **Export** option from the File menu. The Export Data dialog displayed lists the selected spectrum or the spectra in the selected Samples View (Figure 61). You can enter a file name and the destination directory, and then choose the file format the spectra will be exported to.

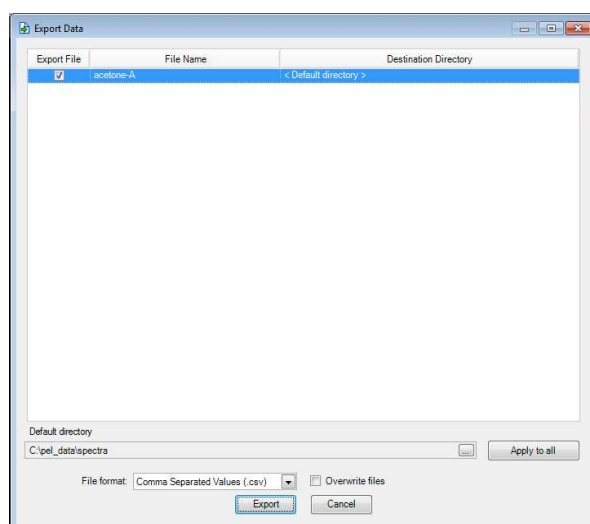


Figure 61 Export dialog

Save ASC

Use the Save ASC option in the graph to save the spectrum as an ASCII file (*.asc). Select a curve and then right-click to display a context menu. Select **Save ASC**, and then browse to a save location.

Send To

The Send To option (Figure 62) sends the contents of the current window to the selected application.



Figure 62 Send To

To see the options on the Send To menu, you must have the appropriate software installed on your PC. To see the Send to Email option, you first need to set up your email account settings on the Setup Email tab.

NOTE: If you cannot see the Word or Excel option, but you do have Microsoft® Office installed on your PC, refer to the *Spectrum Administrator's Guide* (part number L1050095) for troubleshooting information.

You can also use the Send To menu to send your data to Bio-Rad's KnowItAll Informatics System®, if you have the software installed.

To display the Setup Email tab:

- Select **Export and Email** from the Setup menu, and then select the Setup Email tab.

 A screenshot of the 'Setup Email' tab in a software application. The interface is divided into two main sections: 'Server Information' and 'User Information'.

 The 'Server Information' section includes:

- 'Outgoing mail server (SMTP)' with a text box containing 'myserver.net'.
- A checked checkbox for 'Use Default Credentials'.
- An unchecked checkbox for 'Enable SSL'.
- 'Port' with a text box containing '25'.
- Radio buttons for 'Plain Text' (selected) and 'HTML Body'.

 The 'User Information' section includes:

- 'Email Address' with a text box containing 'myemailaddress.com'.
- 'User Name' with an empty text box.
- 'Password' with an empty text box.
- 'Confirm Password' with an empty text box.

 On the right side of the form, there is a 'Test Settings' button. At the top right, there are two tabs: 'Setup Email' (active) and 'Setup Export'.

Figure 63 Setup Email tab

When you select **Send To Email**, the contents of the current window are added to an email form as an attachment. You can then enter the recipient's email address, type your message and add any additional attachments before sending the message.

Reporting

You can generate a report of your data in two ways:

- Using the Report option from the File menu
- Using an Output step in a Macro.

NOTE: Reports are also generated using customized templates for Instrument Verification Checks and Ready Checks. See *Ready Checks and Instrument Verification* on page 87 for more information.

Report

You can generate a report of your results at any time using the **Report** option from the File menu (Figure 64).

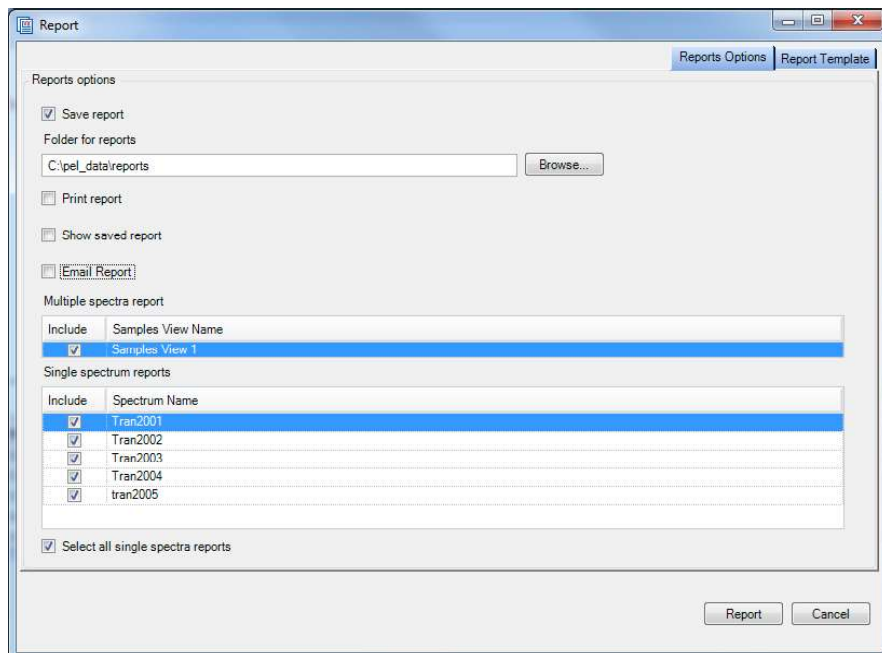


Figure 64 Report dialog

You can generate a report as *.rtf (rich text format) or *.pdf (portable document format) files and then save the report to a file, print it, or attach it to an email.

NOTE: To see the **Email Report** option you must set up your email account settings on the Setup Email tab.

The default **Folder for Reports**, here C:\pel_data\reports, was defined during the software installation. To change the default location, browse to a new folder.

Reports are generated using a template. You can select the sections you want to include in your report on the Report Template tab. The items listed depend on the template selected. In the example shown in Figure 65, we have included the spectrum and the Compare results.

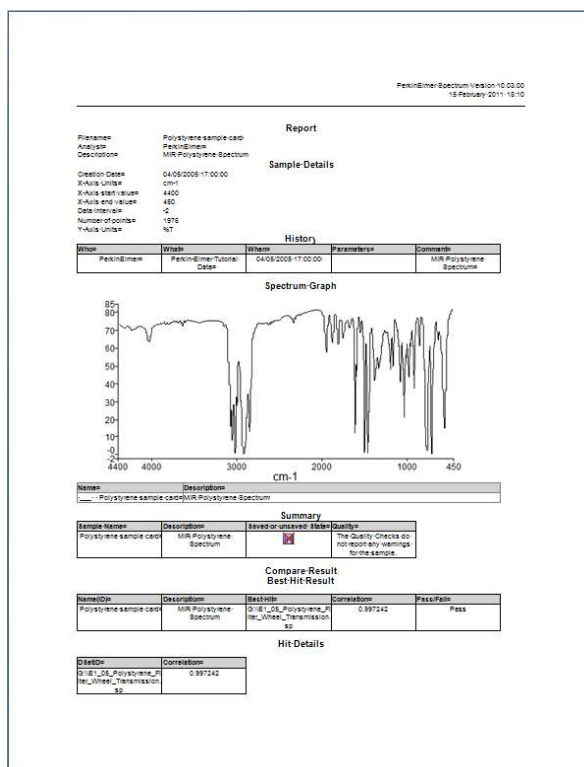


Figure 65 Example report showing Compare result

NOTE: You can also create a report as part of an Output step in a Macro. See the **Macros** tutorial and the Spectrum on-screen help for more information.

Printing

The **Print** and **Print Preview** options from the File menu send the contents of the current window displayed to the printer. Print Preview enables you to change your Page Setup, such as the paper size and orientation, before printing.

NOTE: You can also print your data as a Report.

Instrument Settings

If you want to change any of the default instrument settings, use the Setup Instrument tabs.

- Select **Instrument** from the Setup menu to display the Setup Instrument tabs.
To amend any value, select the parameter and then enter your new value, or select a value from the drop-down list.

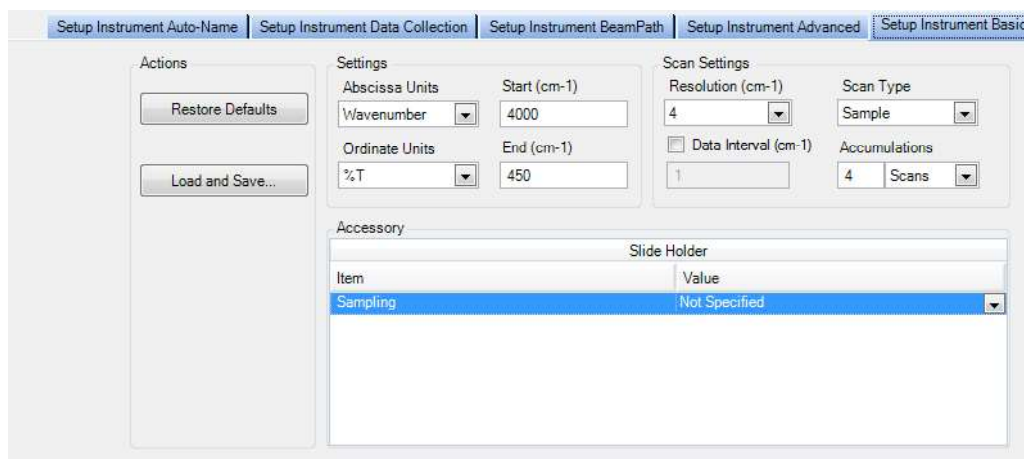


Figure 66 Setup Instrument Basic tab

On the Setup Instrument Basic tab you can set the **Start** and **End** points of the scan range (by default in wavenumbers, but the abscissa units can also be set to nanometers or microns) and the **Accumulations** required, either as a number of scans, or as a length of time. You can also set the **Resolution** (in cm^{-1}).

You can also save and export instrument settings as *.set files for use in an Instrument Setup step in a Macro, or for transferring instrument settings between compatible instruments or between PCs, using **Load and Save** (Figure 66).

Refer to the Spectrum tutorial **Setting Up Your Instrument** for more information on the Setup Instrument tabs, or refer to the appropriate topic for each tab in the Spectrum on-screen Help.

NOTE: The Instrument Settings and Measurement toolbars can be configured to contain any setting available on the Setup Instrument tabs.

Changing the Resolution

The **Resolution** setting is on the Setup Instrument Basic tab in Spectrum software (Figure 28).

The resolution achievable in the instrument is determined by both the optical path difference in the interferometer and the beam divergence in the interferometer as seen by the detector. The Spectrum Two spectrometer has a slot in the double-sided slide holder that enables you to insert a J-stop card before the sample (Figure 67).



Figure 67 The double-sided slide holder

J-stop cards set the upper limit to the resolving power (wavenumber/resolution) of the instrument by limiting the beam divergence. Hence, to achieve a resolution defined by the optical path difference (for example, 2 cm^{-1}), as specified by the **Resolution** on the Setup Instrument Basic tab, a certain beam divergence is required and this is dictated by a given J-stop aperture diameter. J-stop cards are provided with Spectrum Two to enable 4 , 2 , 1 and 0.5 cm^{-1} resolutions at 4000 cm^{-1} .

At a given wavenumber, the smaller the J-stop aperture, the finer the resolving power (assuming we are not limited by the optical path difference scanned by the interferometer). Hence, at 4000 cm^{-1} the 4 cm^{-1} J-stop card has a given diameter to deliver a resolving power of 1000. However, this same diameter may be used to achieve 2 cm^{-1} at 2000 cm^{-1} or 1 cm^{-1} at 1000 cm^{-1} , providing that the optical path difference (set by the **Resolution** setting in the software) is set up appropriately. This can be useful where higher resolution is needed for low-energy situations, where it is only required to achieve resolutions up to lower wavenumber ranges. For example, using a 4 cm^{-1} J-stop to deliver 2 cm^{-1} resolution to 2000 cm^{-1} only can enable higher signal-to-noise to be achieved (or permit shorter scan times) than using the 2 cm^{-1} J-stop card which would deliver 2 cm^{-1} resolution to 4000 cm^{-1} .

For normal operation at 4 cm^{-1} resolution as defined in the software, the Spectrum Two optics are designed to deliver an approximately 4 cm^{-1} instrument lineshape and specified wavenumber calibration without the use of the 4 cm^{-1} J-stop card (assuming the sample is not acting to restrict the beam). However, when highest wavenumber accuracy in direct transmission measurements is required, we recommend use of the optional AVI function with the 4 cm^{-1} J-stop card installed. This ensures the purest lineshapes at higher wavenumbers.

NOTE: This assumes the sample is not restricting the beam and itself forming an effective J-stop. For highest accuracy work, we recommend to always ensure the sample is larger than the J-stop diameter.

If you change the **Resolution (cm⁻¹)** in Spectrum software with the slide holder installed in the sample compartment, a message will be displayed on the Setup Instrument BeamPath tab, and in the Status Bar, prompting you to insert one of the J-stop cards in the slide holder, or to remove any external J-stop card (Figure 68).

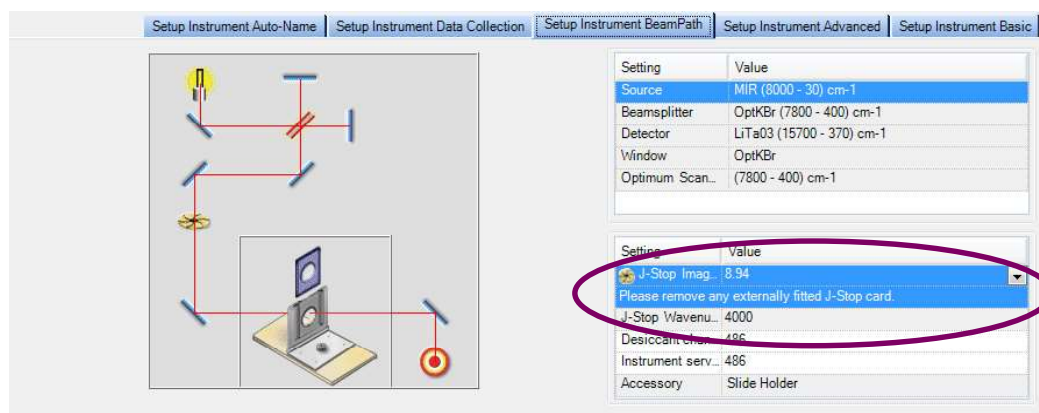


Figure 68 Setup Instrument BeamPath tab

The J-Stop size selected and the Resolution will be recorded as part of the Instrument Settings on the History tab of the spectrum. See the Spectrum on-screen help for more information.

NOTE: For accessories other than the Slide Holder, you cannot insert a J-stop card. Therefore, increasing the resolution (resolution values below 2 cm⁻¹) decreases the J-Stop Wavenumber, the maximum wavenumber at which you can achieve that resolution.

Component Checks

The Component Checks are run automatically the first time you connect to the instrument. You can select to run component checks each time you connect to the instrument, on demand, or after a scheduled number of days on the Setup Laboratory Actions tab in the Laboratory Scheduler. Refer to the Spectrum on-screen Help for details.

To run the Component Checks on demand:

- Select **Component Checks** from the Instrument Checks sub-menu on the Measurement menu.

The Component Checks dialog is displayed (Figure 69) and the tests are run. Each item is assigned a pass ✓ or fail status ✗. If the Component Checks identify a problem, further information or instructions will be provided in the Recommended Action section.

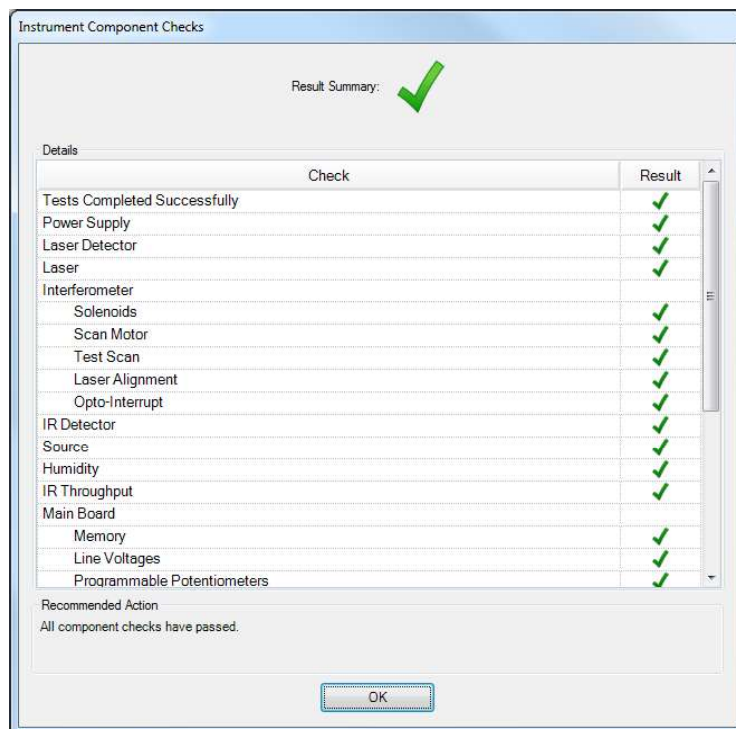


Figure 69 Component Checks dialog

If the Component Checks identify that a user-maintainable part needs to be replaced, for example the source or desiccant, a link to the appropriate Replacement Wizard will be displayed (Figure 70). The Replacement Wizard will provide step-by-step instructions for replacing the part. Refer to the relevant section in *Maintenance*, starting on page 95, for more information.

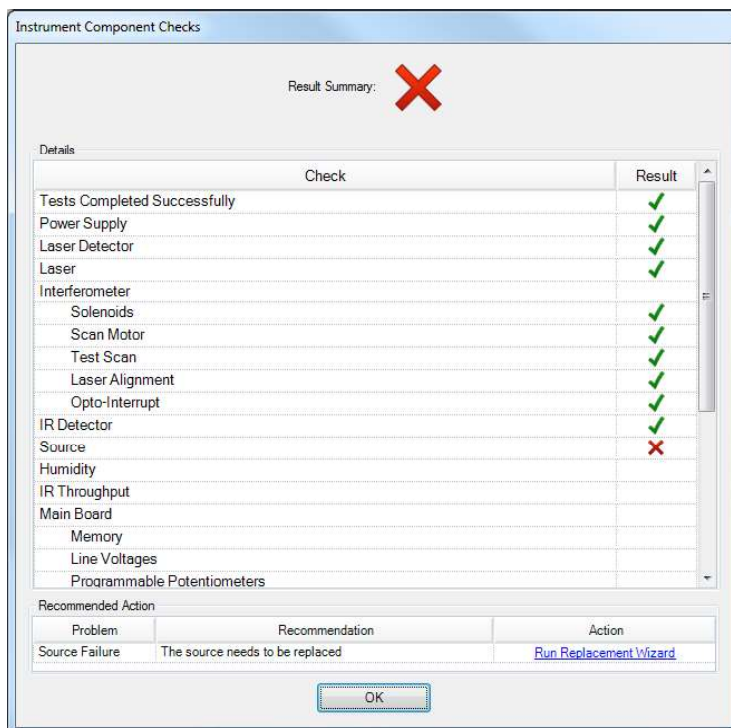


Figure 70 Component Checks dialog with source failure

If the Component Checks identify a problem that may require investigation by a PerkinElmer Service Representative, refer to www.perkinelmer.com/SpectrumTwoSupport for assistance.

If your PerkinElmer Service Engineer requires the log files created during the Component Checks, these are located at:

- C:\ProgramFiles\PerkinElmer\ServiceIR\Component Checks\[Instrument Serial Number]
- OR
- C:\ProgramFiles (x86)\PerkinElmer\ServiceIR\Component Checks\[Instrument Serial Number]

for Windows XP/Windows 7 (32-bit) or Windows 7 (64-bit), respectively, where "C:" is the drive on which Spectrum software is installed.

Humidity Shield

The humidity shield displays the current internal humidity of the spectrometer as measured by the humidity sensor inside the instrument.

- Select **Humidity Shield** from the Measurement menu.
The Humidity Shield dialog is displayed.



Figure 71 Humidity Shield

The information your humidity shield may display is listed in Table 3.

Table 3 Humidity Shield status information

Status	Appearance	Humidity Range	Action Required
Normal	0%	<10%	No action is required.
High	20%	20–39%	Desiccant change is recommended.
Critical	40%	≥40%	Replace the desiccant immediately to avoid instrument damage.

If the humidity of your instrument reaches high or critical levels, the humidity sensor will display a warning message on the Status bar.



Figure 72 Humidity sensor High and Critical warning messages

NOTE: The humidity is also checked during the Component Checks.

The expiry date of the desiccant is based on the date the desiccant was last changed. It gives an indication of when the desiccant is expected to expire in normal conditions (up to five years). However, if your spectrometer is used or stored in an environment that has high levels of humidity you are advised to use the Humidity Shield to check the humidity of your instrument more frequently.

To replace your desiccant you must use the Desiccant Replacement Wizard:

➤ Click **Replace desiccant**.

Follow the instructions on-screen. See *Changing the Desiccant* on page 98 for more information.

Power Save Mode

There are two ways you can put the instrument into a low-power mode: by pressing the power button on the front of the instrument or using the Power Save option in Spectrum software.

Using the button on the front of the instrument

To put the instrument in low-power mode:

- Press the Power On button on the front of the instrument (Figure 73) for approximately 2 seconds until the LED turns from solid green to solid yellow.
If you are connected to the instrument in Spectrum software, the Setup Instrument tabs Measurement menu and the Scan toolbars will be disabled.



Figure 73 Power button on the instrument

NOTE: If you use the Power button to put the instrument in low-power mode, the instrument will not be under software control. Consequently, any scheduled Power Save mode event in Spectrum software will not occur until after you have manually repowered the instrument.

To power up the instrument again:

- Press the Power button on the front of the instrument for approximately 2 seconds until the LED turns green.
The instrument will take a couple of minutes to initialize. When the initialization is complete, and if you were connected to the instrument previously, the Setup Instrument tabs and Scan toolbars will be available.

Using Power Save Mode in Spectrum software

You can use the Power Save option in Spectrum software to control when the instrument is in standby or powered up. You can set up the Power Save options independently for each day of the week.

- Select **Laboratory Scheduler** from the Setup menu, and then select the Setup Power Save tab (Figure 74).

Enter the Power On and Power Off times for each day.

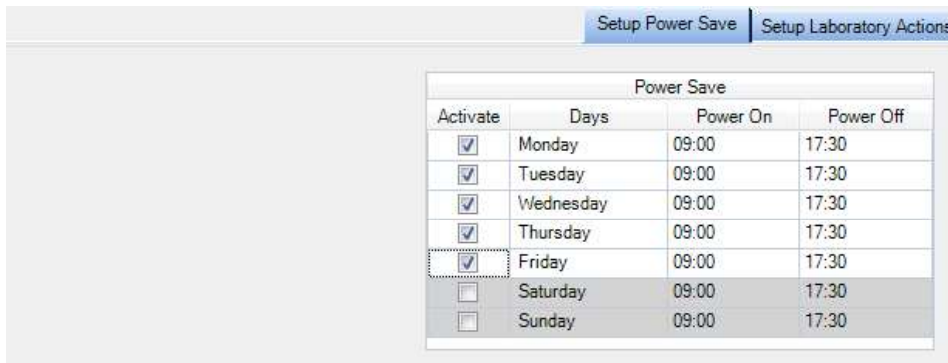


Figure 74 Setup Power Save tab

The instrument will enter Power Save mode at the scheduled time.

NOTE: Shortly before the instrument enters Power Save mode, a message will be displayed. You then have the option to postpone the event for up to 2 hours.

The instrument's internal clock is synchronized with the last PC to make a connection. To update the clock, either after manually changing the PC time, or after an event such as Daylight Savings Time, connect to the instrument using either Spectrum, Spectrum ES or AssureID.

To put the instrument in Power Save Mode at any time:

- Select **Power Save Mode** from the Measurement menu.

During Power Save

When the instrument is placed in Power Save Mode the LED on the front of the instrument will flash yellow to indicate that the instrument will start up again at the scheduled time.

Power on event

At the scheduled time, or if the Power On button is pressed, the LED turns from flashing yellow to solid green. The instrument will then take a couple of minutes to initialize. When the initialization is complete, and if you were connected to the instrument previously, the Setup Instrument tabs and Scan toolbars will be available.

NOTE: If you use the Power button on the front of the instrument to put the instrument in low-power mode, the instrument will not be under software control. Consequently, any scheduled Power Save mode event in Spectrum software will not occur until after you have manually repowered the instrument.

Ready Checks and Instrument Verification

There are three types of Instrument Checks in Spectrum software (Figure 75):

- Component Checks, which check that the components of your instrument are working. For more information refer to *Component Checks* on page 81. You are advised to run these each time you start your instrument.
- Ready Checks, which check that your system – that is, instrument and accessory – are fit-for-purpose. You are advised to run appropriate Ready Checks before starting your sample analysis. For the Contamination Check, this would be before preparing each sample. A Ready Check is specific to the current instrument configuration.
- Instrument Verification, which provides basic checks to determine that your instrument is performing within parameters. These tests should be performed according to the working practices of your laboratory, but usually weekly, or monthly, would be appropriate.

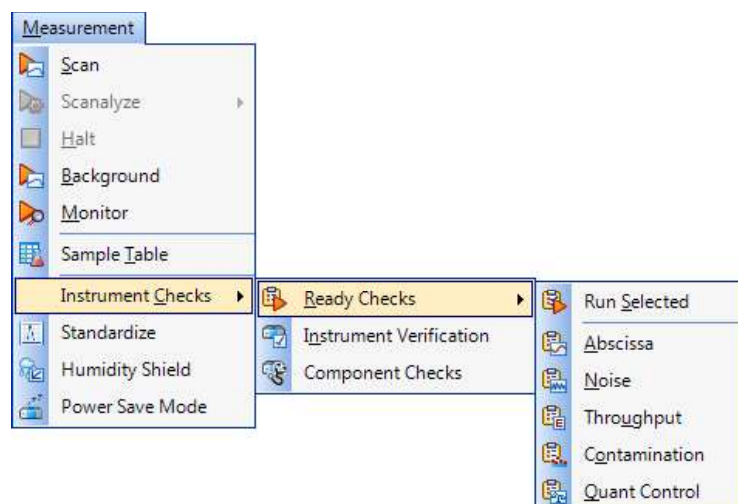


Figure 75 Instrument Checks sub-menu of the Measurement menu

Ready Checks

A Ready Check demonstrates that an aspect of the performance of your complete system, including sampling accessory, is fit-for-purpose. When defining tolerances for Ready Checks, you should consider what the definition of that is for your individual application.

- To run the tests, select **Instrument Checks** and then **Ready Checks** from the Measurement menu, and then select the Ready Check you want to run.
You can run the ready checks individually or run all the Ready Checks selected on the Setup Ready Checks tab using the **Run Selected** option. Follow the instructions on-screen.

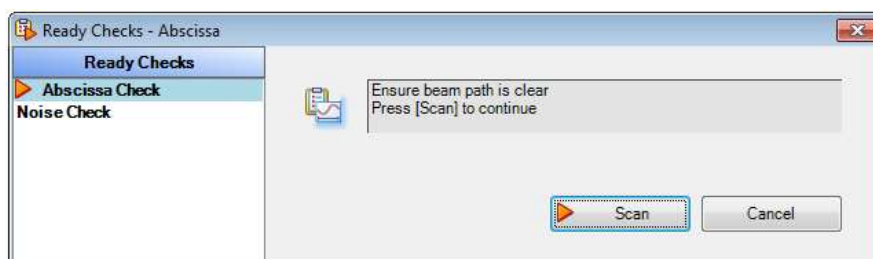


Figure 76 Ready Checks dialog

- The Contamination Check is applicable to sampling accessories that include a component, such as a top plate, that may require cleaning between samples. This includes the UATR and HATR accessories. The check compares a background spectrum taken after your sample has been removed with a reference background spectrum taken when the accessory was perfectly clean. The ratioed spectrum is then examined in absorbance for any sample residue.
You require a suitable reference background spectrum and can enter details for up to three peaks that are characteristic of the possible contaminant.
- The Quant Control Check enables you to verify your Quant Method before scanning your samples. The concentration of a control sample is calculated using the Quant Method, and compared with the known concentration. If it is within limits defined during setup, the check passes.
- The Abscissa Check collects a background spectrum and then collects the spectrum of a polystyrene reference sample (either using the polystyrene reference in the filter wheel, or a polystyrene reference inserted in the slide holder). It then measures the wavenumber at the specified peaks. If the wavenumber value is within the tolerances defined during setup, the check passes.
- The Throughput Check collects a spectrum and measures the ordinate value at each of the specified abscissa positions. If the measured ordinate value is above the lower limit, the check passes.
- The Noise Check collects two background spectra and then measures the RMS (%T) and Peak-to-Peak (%T) noise over a range and report the baseline Trend. If the values are within limits defined during setup, the check passes.

At the end of the tests a report will be generated (by default) containing the results.

Refer to the Spectrum on-screen help for more information on setting up Ready Checks.

Instrument Verification

You can run the basic Instrument Verification Checks without changing any settings. However, you can select further tests and modify the default values for each test.

NOTE: Before performing any Instrument Verification tests you should remove any sampling accessory from the beam path. If your instrument does not have an internal filter wheel, then you will need the slide holder inserted in the beam path.

- To run the tests, select **Instrument Checks** and then **Instrument Verification Checks** from the Measurement menu.
Follow the instructions on-screen.

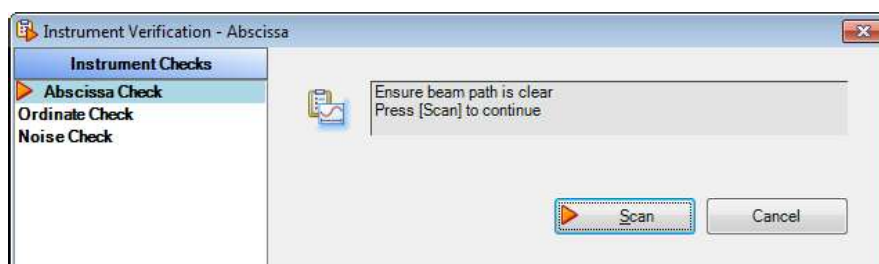


Figure 77 Instrument Verification dialog

The Abscissa Check collects a background spectrum and then collects the spectrum of a polystyrene reference sample (either using the polystyrene reference in the filter wheel, or a polystyrene reference inserted in the slide holder). It then measures the wavenumber at the specified peaks. If the wavenumber value is within the tolerances defined during setup, the check passes.

The Ordinate check by default uses the NG11 Schott Glass (either using the NG11 reference in the filter wheel, or a polystyrene reference inserted in the slide holder). You can choose another reference material for the tests, but you will need to change the default settings.

The Noise Check collects two background spectra and then measures the RMS (%T) and Peak-to-Peak (%T) noise over a range and reports the baseline Trend. If the values are within limits defined during setup, the check passes.

At the end of the tests a report will be generated (by default) containing the results.

You can run up ASTM Level 0 tests, or tests that comply with the requirements of several national pharmacopoeias. Refer to the Spectrum on-screen help for more information on setting up Instrument Verification Checks.

Atmospheric ($\text{CO}_2/\text{H}_2\text{O}$) Suppression

Atmospheric suppression, selected by default on the Setup Instrument Advanced tab (Figure 78), is an atmospheric correction routine.

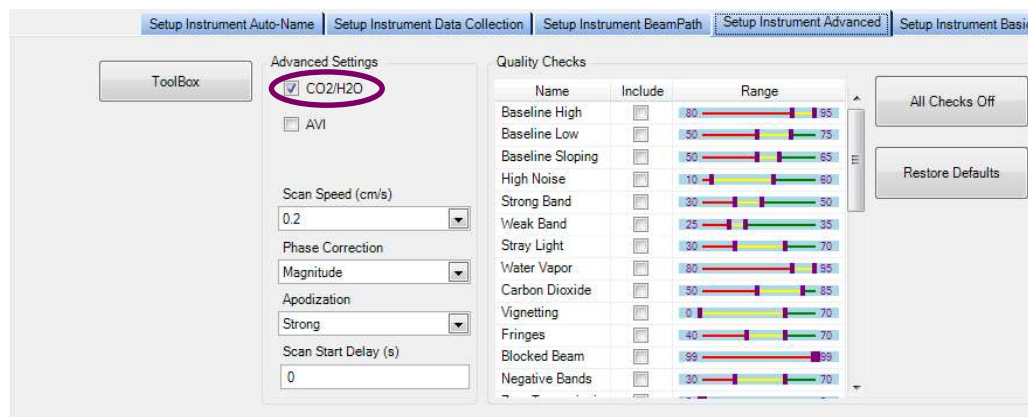


Figure 78 Setup Instrument Advanced tab in Spectrum

This routine is more powerful than simple subtraction, overcoming the following issues:

- Non-linearity due to resolution
- The measured spectrum is temperature dependent
- Lineshape and calibration are affected by J-stop and sample or accessory.

When **CO2/H2O** is switched on, the software uses a single reference spectrum derived from high-resolution data and our understanding of the instrument to model the lineshape, then finds the current real instrument parameters by least-squares fitting to the measured spectrum.

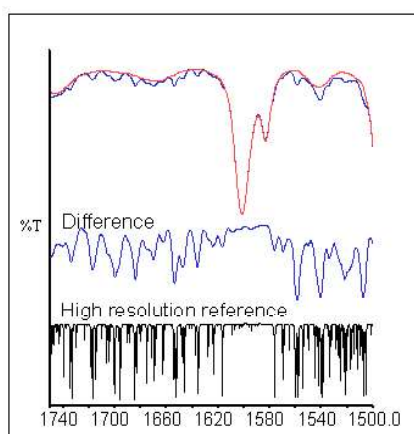


Figure 79 Correction of an MIR spectrum at 4 cm^{-1} resolution

AVI Correction

If available for your current instrument and sampling configuration, AVI correction can be selected on the Setup Instrument Advanced tab in Spectrum (Figure 80).

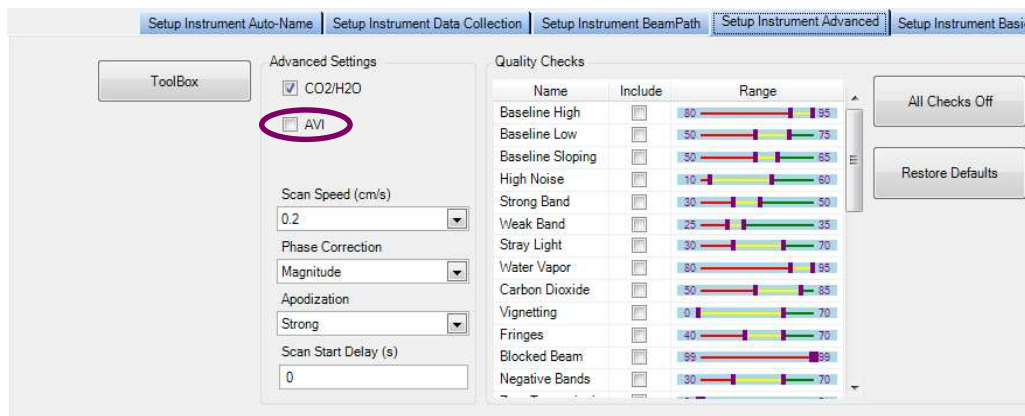


Figure 80 Setup Instrument Advanced tab in Spectrum

The objectives of Absolute Virtual Instrument (AVI) correction are:

- Consistent performance over time and between instruments
- Traceability for all measurements.

Although FT-IR spectrometers use a reference laser, the wavenumber calibration and lineshape are affected by differences in beam divergence and uniformity. This is true for all FT-IR spectrometers. Differences can occur between instruments, when using different sampling accessories and when components are changed. AVI enables calibration and lineshape to be maintained.

The Absolute Virtual Instrument is an instrument with theoretical performance, such that the result of measuring a known sample on such an instrument can be predicted. So, if we measure with a real instrument and calculate the software transform to match the theoretical result, we can apply this transform to future measurements.

The Absolute Virtual Instrument is defined by wavenumber calibration, instrument lineshape and ordinate accuracy.

When **AVI** is switched on, the software measures the current instrument profile relative to an absolute standard (a methane cell) and an ideal lineshape function, and applies a correction.

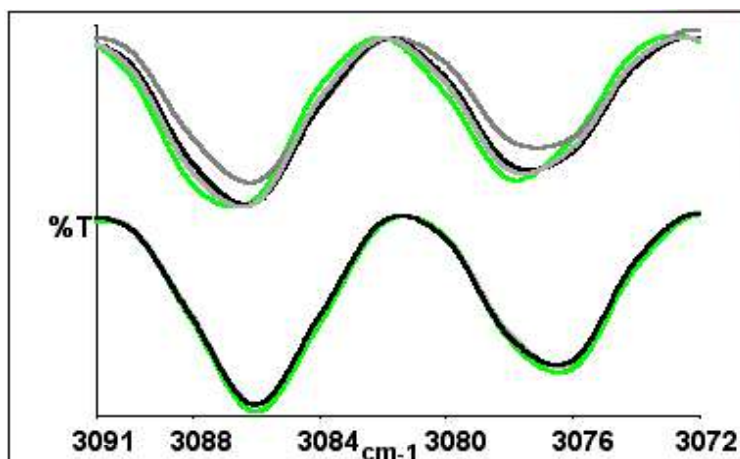


Figure 81 Spectra of methane at 4 cm^{-1} resolution as measured (top) and with AVI (bottom)

AVI correction can only be performed if an AVI Calibration has been set up for the current configuration and resolution.

AVI Calibration

NOTE: AVI calibration uses a methane gas cell (part number L1250462) inserted in the slide holder. It is particularly useful for highest accuracy quantitative transmission measurements. You will not be able to perform an AVI correction if you have a sampling accessory, for example a universal ATR, installed in the sample compartment.

To set up an AVI Calibration:

- Select **Standardize** from the Measurement menu.

OR

Select **AVI** from the **Adjustments Toolbox**, accessed via the Setup Instrument Advanced tab.

Follow the instructions on-screen. For further information, refer to the Spectrum on-screen Help file.

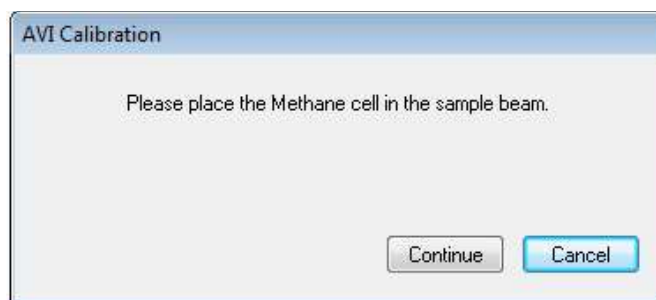


Figure 82 AVI Calibration dialog prompting the user to insert the methane cell

Exit Spectrum Software

When you exit Spectrum software you can choose a Save Option appropriate for what you want to do next time you use Spectrum.

If you want to continue working with the same data, or to collect more samples listed in your Sample Table, you can resume your session next time with all your data loaded. If you choose not to reload your data, you can make sure that any unsaved data is saved to the appropriate default location you chose at installation.

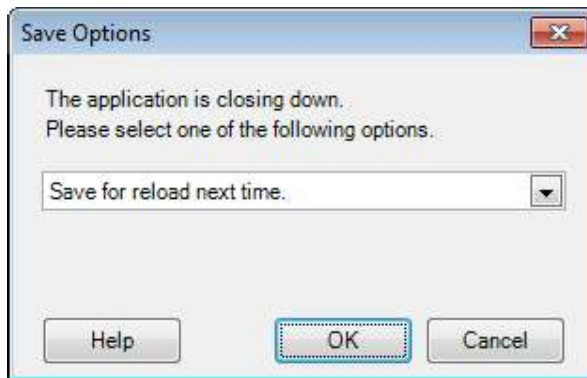
To exit Spectrum:

1. Select **Exit** from the File menu.

OR

Click the  at the top right of the Spectrum window.

The Save Options dialog is displayed.

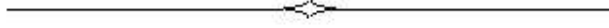


2. Select whether to:

Save unsaved datasets – save any unsaved data, and open Spectrum with your default settings and layout next time, which enables you to preserve your current workspace for when you next log on to Spectrum at this PC.

Save for reload next time – save any unsaved data, and reload the current spectra, settings and layout next time, which enables you to carry on with your work from where you left off when you next log on to Spectrum at this PC.

Exit without saving datasets – exit without saving any unsaved data, layout or settings information, which restores the default workspace when you next log on to Spectrum at this PC.



Maintenance

Overview

This section covers the maintenance that can be carried out by a user.

It describes:

- Cleaning the spectrometer
- Replacing the desiccant
- Purging the sample area
- Purging the instrument optics
- Replacing the sample compartment windows
- Replacing the source
- Replacing the main board air filter.

NOTE: You *must* use the appropriate Replacement Wizard in Spectrum, Spectrum ES or AssureID software to replace the source, desiccant or sample compartment windows, as described in this section. During the maintenance procedure, the internal temperature of the instrument is maintained to prevent the ingress and condensation of water vapor, which could damage the optics.

Cleaning the Spectrometer

Clean the outside of the instrument using a damp cloth. If necessary, a mild detergent may be used. Before you clean the entire instrument, always perform a patch test on an inconspicuous area.

Avoid spilling liquid into the instrument. Clean all external spills immediately.

Changing the Desiccant

Expect to change the desiccant in the spectrometer approximately every five years. Old, used desiccant releases moisture.

CAUTION

In regions experiencing high humidity levels we recommend that you change the desiccant more often, and that you monitor the internal humidity of your instrument using the Humidity Shield (refer to page 83) regularly.

The desiccant change interval is set in the **Desiccant change due in (days)** option on the Setup Instrument BeamPath tab in Spectrum software (Figure 83).

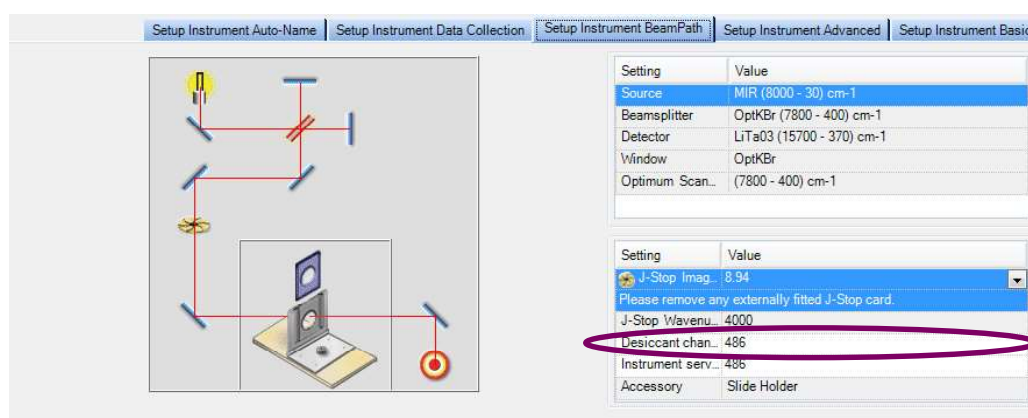


Figure 83 Setup Instrument BeamPath tab in Spectrum

If the desiccant change due date has passed, a warning will be displayed in the Status Bar and in the table on the Setup Instrument BeamPath tab.

The warning is displayed until you update the software that the desiccant has been changed. To reset the desiccant change interval, select the current value, click **Changed** to clear any warning messages.

You may also be prompted to change your desiccant during the Component Checks.

To replace the desiccant, you will require the desiccant replacement kit (part number L1600244). The kit contains a wrench and two bags: one large and one small.

Inspect the humidity indicator card in the plastic bag containing the larger of the two bags. If the card is pink it indicates moisture in the bag, and you should discard the desiccant pack. Only use the replacement desiccant bag if the indicator is blue.

CAUTION

Old, used desiccant releases moisture and can cause high humidity levels inside the instrument resulting in catastrophic failure of KBr optics.

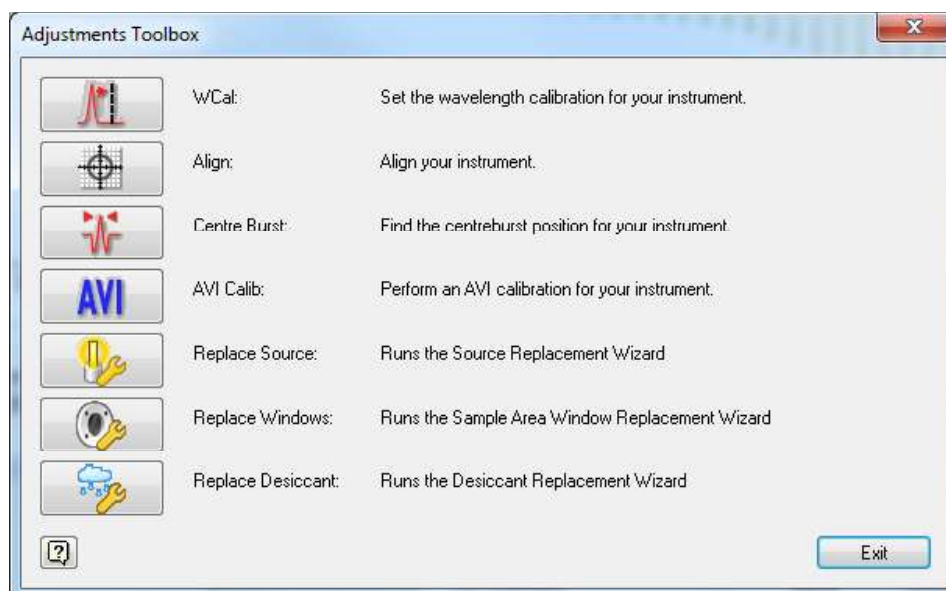
Do not use damaged packs of desiccant. Make sure that the packs you use have not been left in contact with the air.

The instrument must be switched on and you must be connected to the instrument in Spectrum, Spectrum ES or AssureID software. You can start the Desiccant Replacement Wizard from the Adjustments Toolbox or, if the Component Checks identify high humidity as a problem, by selecting **Run Desiccant Replacement Wizard** on the dialog. You can also start the wizard by clicking **Replace desiccant** on the Humidity Shield dialog.

NOTE: In AssureID software, the **Adjustments Toolbox** is available from the **Configure Instruments and Accessories** group on the Tools menu.

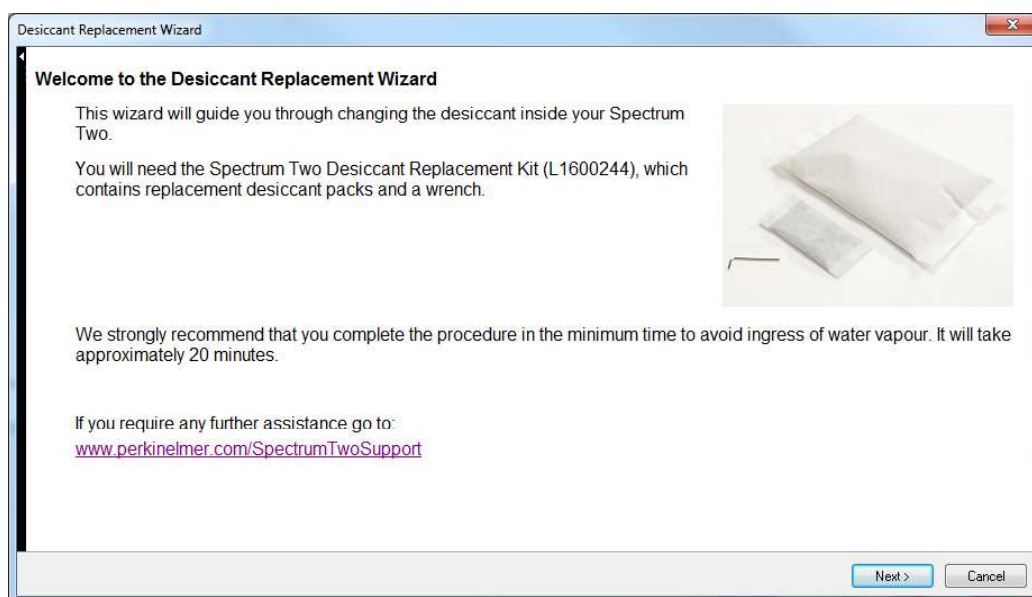
To replace the desiccant when connected to Spectrum software:

1. Select **Instrument** from the Setup Menu.
The Setup Instrument tabs are displayed.
2. Select the Setup Instrument Advanced tab and then click **Toolbox**.
The Adjustments Toolbox dialog is displayed.



3. Click  .

The Desiccant Replacement Wizard is displayed.



4. Follow the instructions on-screen.

When you have completed the procedure the **Desiccant change due in (days)** is reset automatically to **1800** days.

Purging the Spectrometer

Purge the sample compartment if you need to make sure that no residual water vapor or CO₂ peaks are visible in the spectrum. The connectors are on the underside of the instrument (Figure 84).

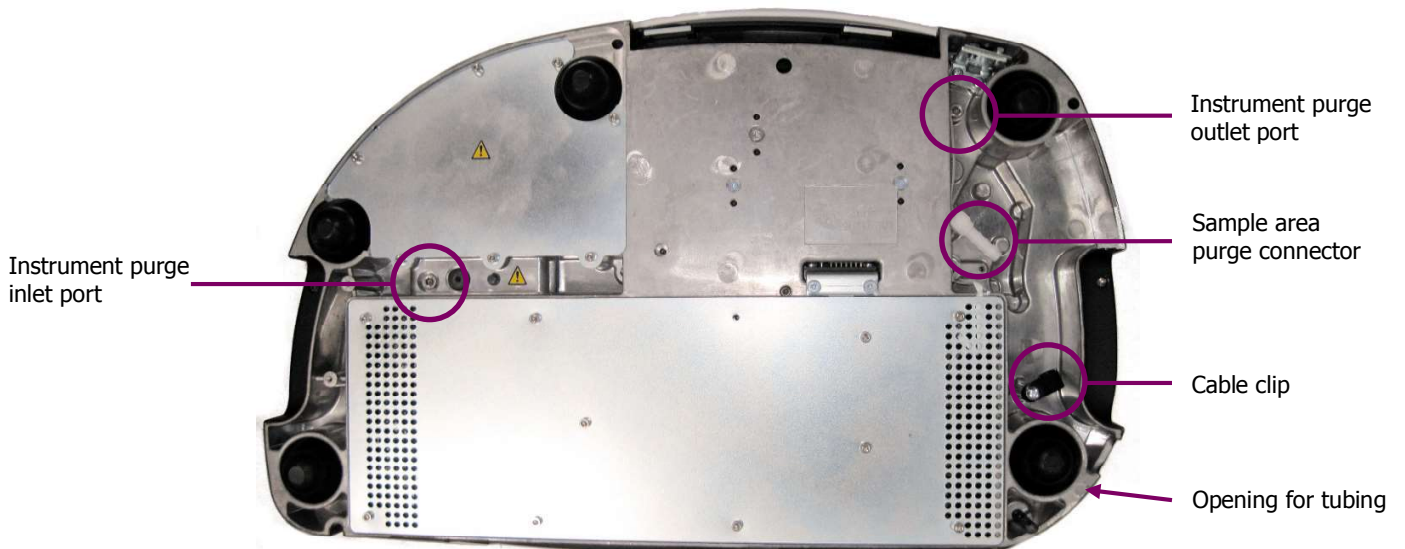


Figure 84 Location of purge connectors

Although connections are provided, under most circumstances you should not purge the optical system. The Spectrum Two instrument was purged and then sealed after manufacture. To purge the instrument you will need to break the seal on the instrument, which will invalidate your instrument warranty.

You can purge with either dry air or nitrogen. Both remove water vapor; however, nitrogen is preferable because it also removes atmospheric carbon dioxide.

A typical cylinder of dry nitrogen (or dry air) stores 6.26 m³ at 1.4 × 10⁴ kPa (220 ft³ at 2200 lbf/in²). Make sure that the gas is free of oil, water, or dirt particles larger than 25 μm (0.001 inch).



WARNING

Do not site the instrument in a poorly ventilated area if nitrogen will be used as a purge gas.

Oxygen depletion in an enclosed space does not trigger a gasping reflex, and errors of judgment, confusion, or unconsciousness can occur in seconds and without warning.



WARNING

Do not use a flammable gas to purge the instrument. The spectrometer contains a hot source, and a fire or explosion will result. Only use clean, dry, oil-free nitrogen or air to purge the instrument.



WARNING

Never connect the purge tubing directly to a gas cylinder or other high pressure supply; always use a pressure regulator and set the pressure to a maximum of 6.9 kPa (1 lbf/in²) before you start the flow.

Purging the sample compartment

A length of clear plastic tubing (1/4 inch internal diameter, part number L1600245) is provided to transfer the gas to the sample compartment purge connector.

To connect the sample compartment purge:

1. Disconnect from the instrument in your software, if applicable.
2. Disconnect the instrument from the mains power and then remove any cables connected to the rear of the spectrometer.
3. Remove any sampling accessories installed in the sample compartment. You will need to invert the instrument.
4. Carefully, turn the instrument over to display the underside, placing the instrument on a soft surface.
5. Locate the sample compartment purge connector shown in Figure 85.



Figure 85 Sample compartment purge connector

6. Feed the tubing through the opening in the instrument baseplate, through the tubing clip and then push the end of the tubing onto the barbed purge connector.
7. Connect the free end of the tubing to the gas regulator.

NOTE: Ensure the regulator is set to a pressure not greater than 6.9 kPa (1 lbf/in²).

8. Open the gas flow valve on the regulator until a flow rate of 4 L/minute (0.14 ft³/minute) is achieved. It will take about 2 minutes to fully purge the sample compartment.
9. When you have finished work, turn off the gas supply.
10. Disconnect the fitting from the instrument, if required, by easing the tubing off the purge connector.

Purging the instrument

CAUTION

The Spectrum Two instrument was purged and then sealed after manufacture. The bolts in the instrument purge connection ports are marked with tamper-proof paint. If you break the seals on the instrument you will invalidate your instrument warranty. DO NOT proceed unless you fully understand the implications of doing so.

In normal operation it should not be necessary to purge the instrument.

To connect the instrument purge you will need the optional Instrument Purge Kit (part number L1600234). The kit contains tubing, two extenders and right-angled connectors, pliers and two blanking plugs to block the connectors when you have finished purging.

1. Disconnect from the instrument in your software, if applicable.
2. Disconnect the instrument from the mains power and then remove any cables connected to the rear of the spectrometer.
3. Remove any sampling accessories installed in the sample compartment.
You will need to invert the instrument.
4. Carefully turn the instrument over to display the underside, placing the instrument on a soft surface.
5. Locate the instrument purge inlet port shown in Figure 86.
6. Using an M5 hexagonal key, unscrew and remove the bolt in the inlet port (Figure 86).
Retain the bolt for future use.

NOTE: The custom bolts contain an o-ring seal.

Instrument purge
inlet port

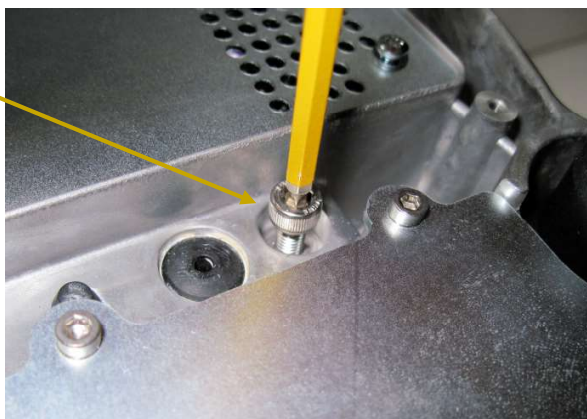


Figure 86 Instrument inlet purge port securing bolt

7. Screw one of the straight connectors supplied into the instrument purge inlet port and tighten using the pliers supplied with the kit (Figure 87).



Figure 87 Instrument purge inlet port straight connector

8. Screw one of the right-angled connectors supplied into the inlet port and tighten using the pliers (Figure 88).



Figure 88 Tighten the purge port right-angled connector

9. Cut the tubing supplied into pieces of suitable length.
10. Push the end of one piece of tubing onto the right-angled connector as shown in Figure 89.

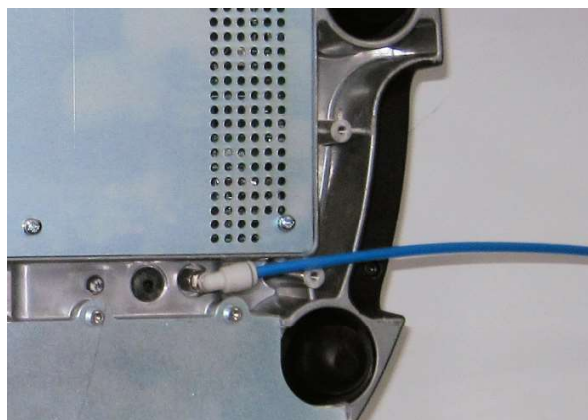


Figure 89 Tubing connected to instrument purge inlet port

11. Connect the free end of the inlet tubing to the gas regulator.

NOTE: Ensure the regulator is set to a pressure not greater than 6.9 kPa (1 lbf/in²).

12. Repeat steps 6–10 to connect the other piece of tubing to the instrument purge outlet port (Figure 90).

Although you *must* remove the bolt from the outlet port before passing gas through the inlet port, it is not necessary to connect the outlet tubing if you do not need to vent the gas outside the operating environment.

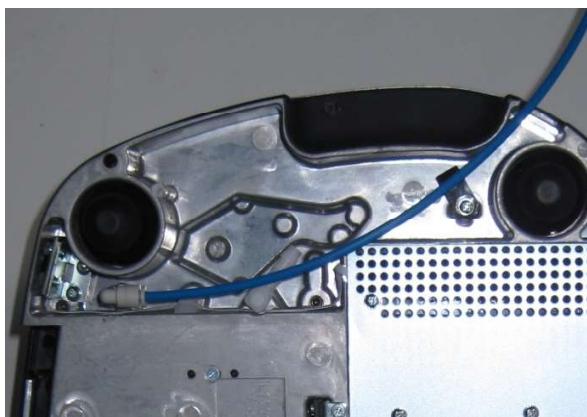


Figure 90 Tubing connected to instrument purge inlet port

13. Feed the purge outlet tubing through the tubing clip and the outlet port and position it to vent to a suitable location (for example, a fume hood).
14. Open the gas flow valve on the regulator until a flow rate of 2 L/minute (0.07 ft³/minute) is achieved.
It will take about 10 minutes to fully purge the instrument optics.
15. When you have finished work, turn off the gas supply.
16. Release the tubing from the instrument purge inlet port and, if fitted, from the purge outlet port.
To release the tubing, pull back the spring fitting on the connector and then gently pull the tubing out.
17. For a temporary seal, fit the blanking bolts supplied into the right-angled connectors.

OR

If you have finished purging your instrument, replace the bolts you removed in Step 6.

NOTE: If you have mislaid the bolts fit the blanking bolts instead, then contact PerkinElmer Customer Care to obtain replacements.

Replacing the Source

If there is a Recommended Action to replace the source in the Component Checks, you will require the source replacement kit (part number L1600243). The kit contains a replacement source and source-doubling mirror assembly, and a 2.5 mm hexagonal wrench.

To replace the source, the instrument must be switched on and you must be connected to the instrument in Spectrum, Spectrum ES or AssureID software. You can start the Source Replacement Wizard from the Adjustments Toolbox or, if the Component Checks identify Source Failure as a problem, by selecting **Run Source Replacement Wizard** on the dialog.

NOTE: In AssureID software, the **Adjustments Toolbox** is available from the **Configure Instruments and Accessories** group on the Tools menu.

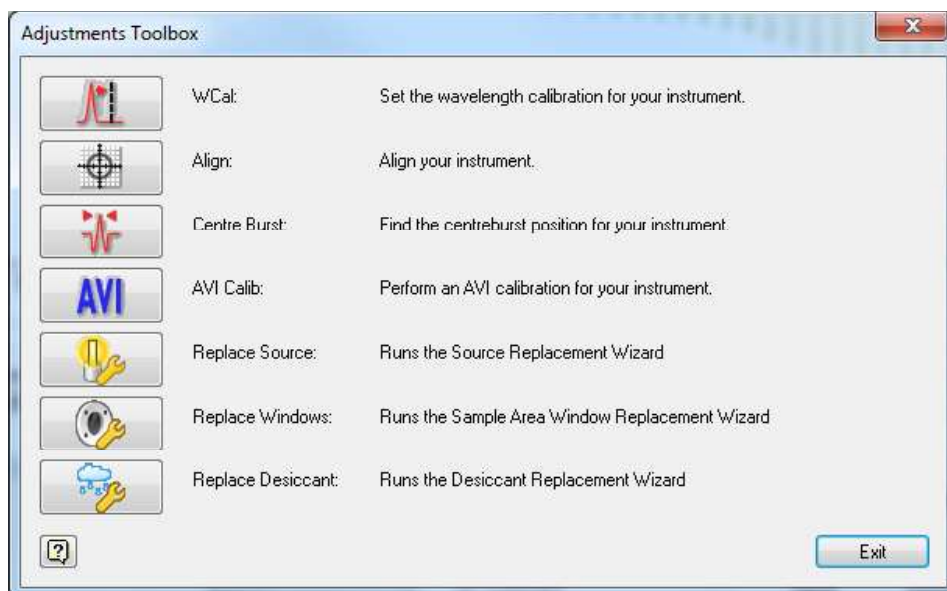
CAUTION

The source element is brittle and can be broken if not handled properly. Be careful when removing and installing the source.

Before starting the source replacement procedure, ensure that you have the source replacement kit available to minimize the amount of time that the source compartment is open.

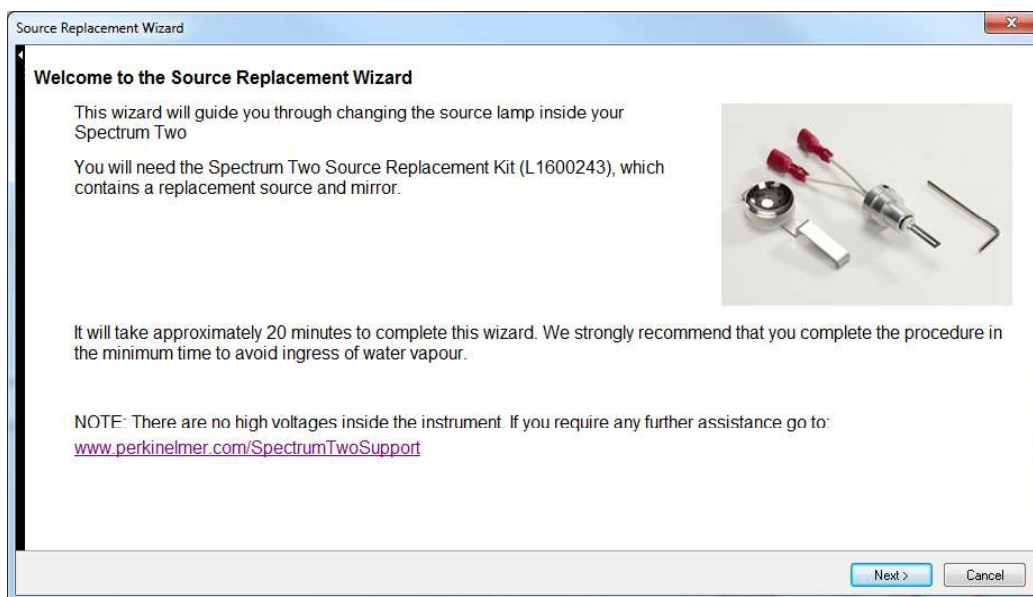
To replace the source:

1. Select **Instrument** from the Setup Menu in Spectrum software.
The Setup Instrument tabs are displayed.
2. Select the Setup Instrument Advanced tab and then click **Adjustments Toolbox**.
The Adjustments Toolbox dialog is displayed.



3. Click  .

The Source Replacement Wizard is displayed.



4. Follow the instructions on-screen.
5. When you have completed the procedure, we recommend that you run the Component Checks to confirm that your instrument is working correctly.
6. Allow the source temperature to stabilize for approximately 2 hours before using the instrument.

NOTE: If you are using the AVI correction, you will need to run a new AVI calibration after replacing the source.

Installing/Replacing Windows

The Spectrum Two spectrometer is available with two types of sample compartment window: KBr for an extended scan range and ZnSe for higher-humidity environments. The hygroscopic KBr windows may become opaque over time. ZnSe windows are not hygroscopic, and you should only need to replace them if they are broken.

To replace the windows you will require the appropriate window replacement kit: part number L1600241 for KBr windows or L1600242 for ZnSe windows. The window replacement kits contain two replacement windows with seals, one for each side of the sample compartment, and a 1.5 mm hexagonal wrench.



WARNING

ZnSe is highly toxic by ingestion. Avoid touching the window material. Handle using the window mounting only.

CAUTION

Be careful not to get moisture on the optical surface of the window. Do not touch or breathe on the optical surface of the window.

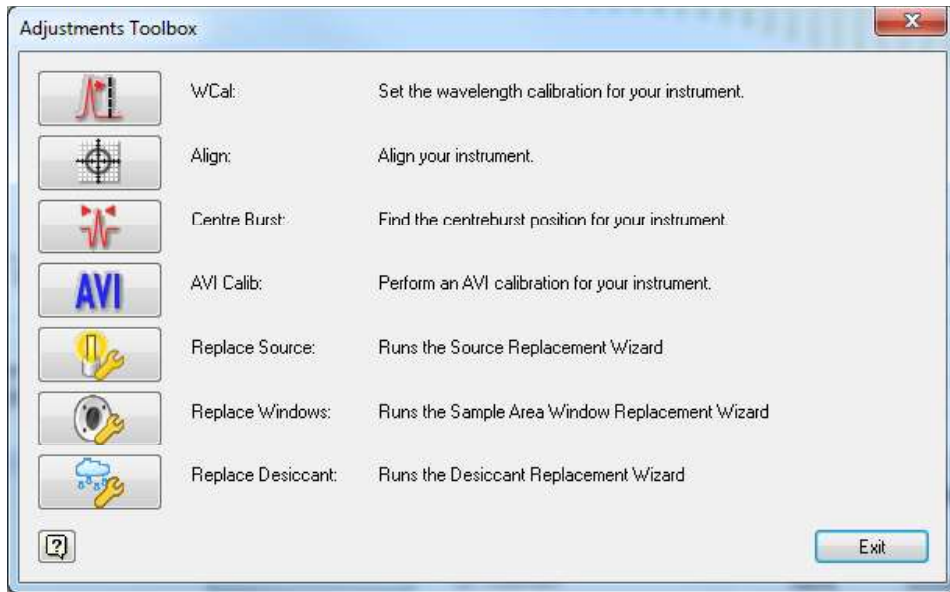
The instrument must be switched on and you must be connected to the instrument in Spectrum, Spectrum ES or AssureID software.

NOTE: In AssureID software, the **Adjustments Toolbox** is available from the **Configure Instruments and Accessories** group on the Tools menu.

To replace the windows when connected to Spectrum software:

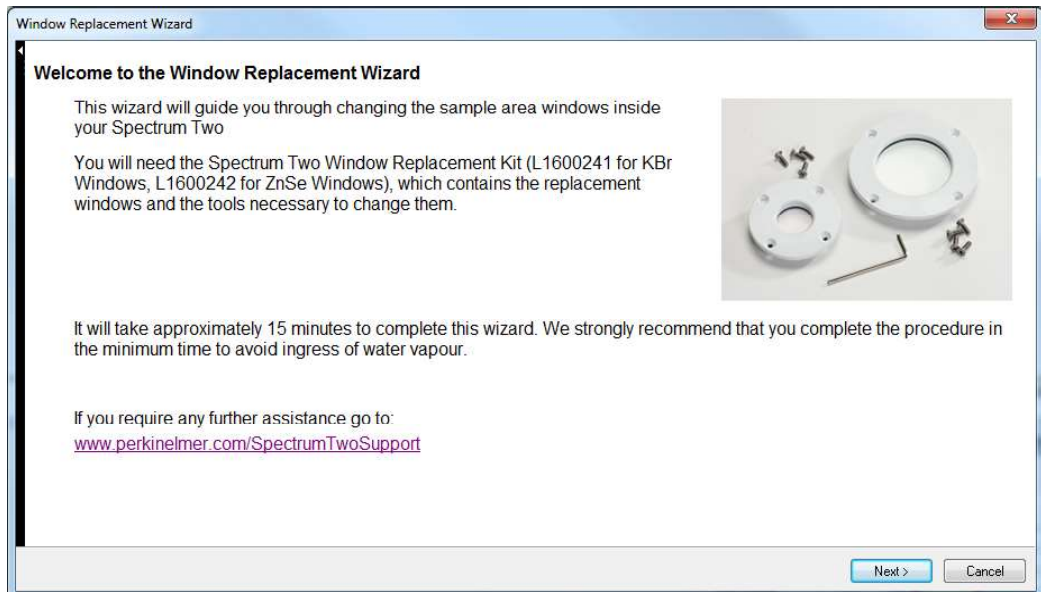
1. Select **Instrument** from the Setup Menu in Spectrum software.
The Setup Instrument tabs are displayed.

- Select the Setup Instrument Advanced tab and then click **Toolbox**.
The Adjustments Toolbox dialog is displayed.



- Click  .

The Window Replacement Wizard is displayed.



- Follow the instructions on-screen.

Replacing the Main Board Air Filter

If your instrument is used regularly in a dusty environment, the main board air filter may become blocked. If it does, you may notice that your instrument takes longer to stabilize. To replace the main board air filter you will need the replacement main board air filter (part number L1601717).

NOTE: Alternatively, the filter is washable in water. Ensure it is thoroughly dry before replacing it in the instrument.

1. Disconnect from the instrument in your software, if applicable.
2. Disconnect the instrument from the mains power and then remove any cables connected to the rear of the spectrometer.
3. Remove any sampling accessories installed in the sample compartment. You will need to invert the instrument.
4. Carefully, turn the instrument over to display the underside, placing the instrument on a soft surface (Figure 91).

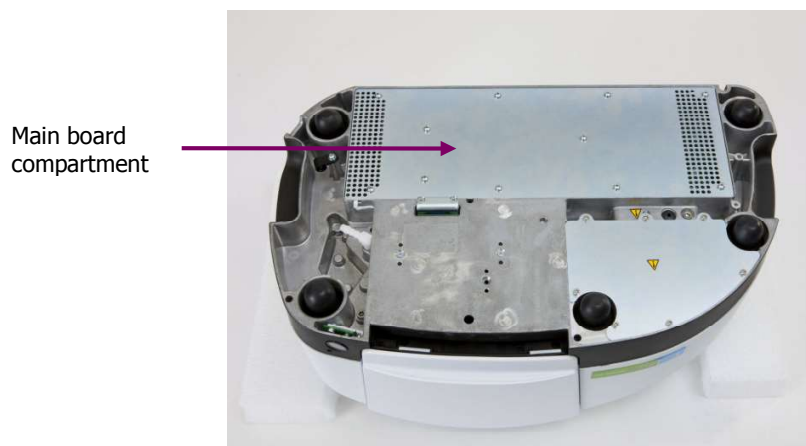


Figure 91 Location of the main board compartment

- Using a Philips-type, PZ No 1 screwdriver, undo the screws securing the main board compartment cover to the instrument and remove the cover (Figure 92). Retain the screws and store in a safe place.

CAUTION

The main board contains static-sensitive devices. Do not touch the main board or electrical components when changing the main board air filter.

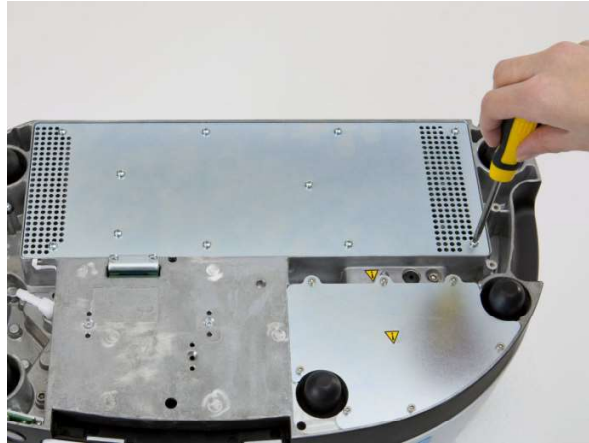


Figure 92 Remove the securing screws

- Locate the used filter (Figure 93).

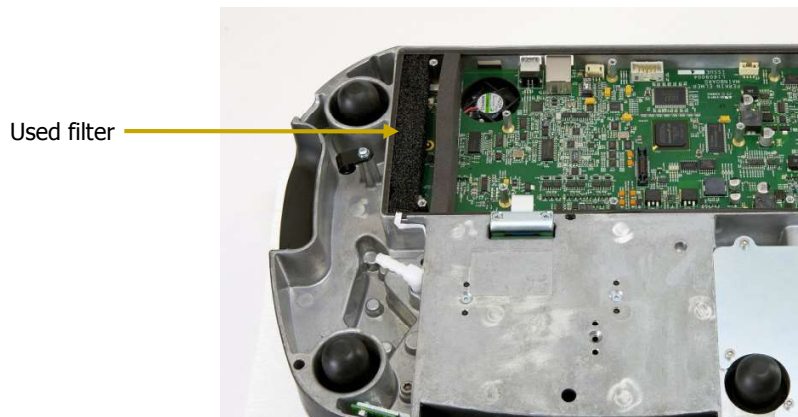


Figure 93 Location of the filter

7. Remove the used filter (Figure 94).



Figure 94 Remove the used filter

8. Slot in the replacement filter, ensuring that it is flat.
9. Replace the compartment cover, and secure with the screws retained in Step 2. Ensure that the white main board cable shown in Figure 95 is not trapped when you replace the compartment cover, but passes through the cut-out in the instrument housing.

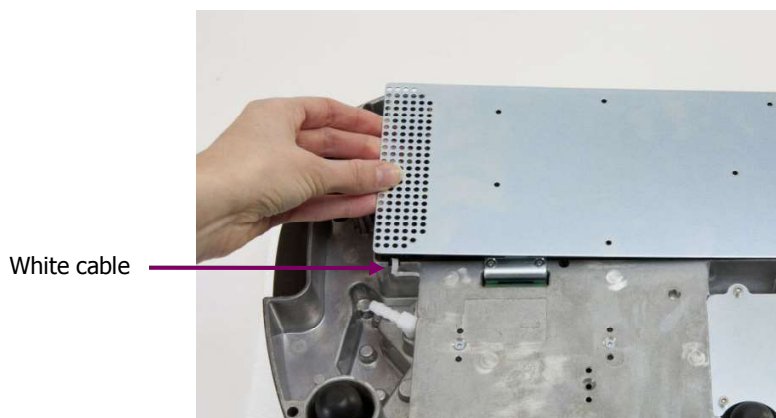


Figure 95 Replace the compartment cover

NOTE: If the compartment cover is not orientated correctly you will not be able to insert all the screws.

Additional Parts

The following optional parts, replacement parts and upgrades are available:

Optional parts

Part Number	Description
L1600238	Spectrum Two Portability Pack
L1600233	Spectrum Two Battery Pack (includes a 12 V car adaptor)
L1600246	Spectrum Two Wireless Router Kit
L9004198	Wireless Dongle
L9004128	Spectrum Two 12 V Car Adaptor
L9004199	Spectrum Two Carry Case
L9004200	Spectrum Two UATR Carry Case.
L1250404	MIR Validation Kit
L1202057	Polystyrene Test Film, 0.038 mm (non-traceable)
L1250462	Methane Test Sample (for AVI)
L1600234	Spectrum Two Instrument Purge Kit
L1600245	Spectrum Two Sample Compartment Purge Kit
L1200466	Ethernet Crossover Cable
L9004196	Barcode Reader
5101188	Crystal Polishing Kit
L1365311	Liquid And Mull FT-IR Sampling Kit
L1365312	General Purpose FT-IR Sampling Kit

Replacement parts

Part Number	Description
L1600243	Spectrum Two Source Replacement Kit
L1600244	Spectrum Two Desiccant Replacement Kit
L1600242	Spectrum Two ZnSe Window Replacement Kit
L1600241	Spectrum Two KBr Window Replacement Kit
L1601717	Spectrum Two Main Board Air Filter
L9004169	USB Cable
L1200466	Ethernet Crossover Cable
L1600232	Spectrum Two J-stop Card Kit
L9002298	Spectrum Two Power Supply
L1600216	Spectrum Two Sample Compartment Lid
L1202057	Polystyrene Test Film (non-traceable)
L1250462	AVI Calibration Methane Cell



Upgrades

Upgrades are installed by a PerkinElmer Service Representative.

Part Number	Description
L1600265	Standard to Temperature-stabilized Detector Upgrade
L1600266	Filter Wheel (APV) Upgrade

Appendices

Appendix 1: Connector Details

	Port	Description	Connector Type	Voltages	Maximum Currents
A	USB 	This is the standard interface between the PC and the instrument.	USB (Type B)	–	–
B	ETHERNET 	100 Base-T Ethernet connector. This is the standard interface between a Local Area Network (LAN) and the instrument. It can also be used to connect direct to the PC.	Ethernet	<5 V	<100 mA
C	EXT DETECTOR	This port enables to you power the optional Wireless Router or connect an external accessory.	Female high-density 15-way d-connector; \pm CAN-bus; i-button	+12 V output	500 mA
				–12 V output	100 mA
				Analog inputs \pm 12 V max. 1K5 ohm	
				0 V	
E	DC Power	The DC power port is used to connect the spectrometer to the power supply. You can use the mains power supply adaptor and cable supplied, or you can use the optional battery pack or car adaptor.		18 V	3 A

Appendix 2: Instrument Performance Validation Kits

The MIR Performance Validation Kit (part number L1250404) contains a polystyrene reference sample and an NG11 Schott Glass reference sample.

Macros are supplied with Spectrum software (version 10.3 or later) that can be used with the Performance Validation kits to produce a report certifying your instrument.

Appendix 3: Decontamination and Cleaning

Before using any cleaning or decontamination methods except those specified by PerkinElmer, users should check with PerkinElmer that the proposed method will not damage the equipment.

Decontamination

Customers wishing to return instrumentation and/or associated materials to PerkinElmer for repair, maintenance, warranty or trade-in purposes are advised that all returned goods must be certified as clean and free from contamination.

The customer's responsible body is required to follow the "Equipment Decontamination Procedure" and complete the "Certificate of Decontamination". These documents are available on the PerkinElmer public website:

<http://las.perkinelmer.com/OneSource/decontamination.htm>

Alternatively, if you do not have access to the internet contact Customer Care:

Customer Care USA: (8:30 a.m. – 7 p.m. EST)	1 800 762 4000 (+1) 203 925 46 02	(inside the USA) (outside the USA)
Customer Care Canada:	800 561 46 46 customercareca@perkinelmer.com	
Customer Care China:	800 820 50 46 customercarecn@perkinelmer.com	
Customer Care EU:	0800 40 858 benelux@perkinelmer.com 0805 111 333 cc.france@perkinelmer.com 0800 181 00 32 cc.germany@perkinelmer.com 0800 90 66 42 cc.italy@perkinelmer.com 8000 99 164 atencionalcliente@perkinelmer.com 080089 60 46 cc.uk@perkinelmer.com	Belgium France Germany Italy Spain UK

If you are located outside these regions, please call your local PerkinElmer sales office for more information.

Cleaning the Instrument

Exterior surfaces may be cleaned with a soft cloth, dampened with a mild detergent and water solution. Do **not** use abrasive cleaners or solvents.

Appendix 4: WEEE Instructions for PerkinElmer Products



A label with a crossed-out wheeled bin symbol and a rectangular bar indicates that the product is covered by the Waste Electrical and Electronic Equipment (WEEE) Directive and is not to be disposed of as unsorted municipal waste. Any products marked with this symbol must be collected separately, and in accordance with the regulatory guidelines in your area.

The objectives of this program are to preserve, protect and improve the quality of the environment, protect human health, and utilize natural resources prudently and rationally. Specific treatment of WEEE is indispensable in order to avoid the dispersion of pollutants into the recycled material or waste stream. Such treatment is the most effective means of protecting the customer's environment.

The requirements for waste collection, reuse, recycling, and recovery programs are set by the regulatory authority at your location. Contact your local responsible person (such as your laboratory manager) or authorized representative for information regarding applicable disposal regulations.

See the PerkinElmer web address below for information specific to PerkinElmer products, and contact details for the Customer care department in your region.

<http://las.perkinelmer.com/OneSource/Environmental-directives.htm>

Products from other manufacturers may also form a part of your PerkinElmer system. These other manufacturers are directly responsible for the collection and processing of their own waste products under the terms of the WEEE Directive. Please contact these manufacturers directly before discarding any of their products.

Consult the PerkinElmer web site (above) for manufacturer's names and web addresses.

Index

A		G	
About This Manual	6	Guided Tour	20
Accessories	25	Communications Ports	23
ATR	25	Optical System	21
Changing	47	Power Switch	23
DRIFT	25	Sample Compartment	21
FASR	26		
HATR	25	H	
Applications Packs	27	HTML help	6
Atmospheric Suppression	95	Humidity Shield	88
AVI			
Calibration	97	I	
Correction	96	Identification	67
C		Compare	68
Cleaning	101	Peak Table	67
External	101	Search	69
Cleaning the Instrument	124	Installation	
CO ₂ /H ₂ O Suppression	95	Connecting to Electrical Supply	37
Communications Ports	23, 35	Connecting to PC (Ethernet)	44
Compare	68	Connecting to PC (USB)	39
Component Checks	86	Connecting to PC (WiFi)	41
Connection Methods	34	Connecting to PC over a Network	
Conventions		(Ethernet)	45
Notes, Cautions and Warnings	7	Instrument Install Wizard	46
Text	7	Software	36
D		Instrument Performance Validation Kits	
Decontamination	124	123
Desiccant		Instrument Settings	83
Changing	102	Instrument Verification	92
E		IPV Kits	123
EMC		J	
Compliance	18	J-stop	
EC directive	18	Changing	84
FCC rules	18	L	
Environmental Conditions	14	Labels	
Equations	74	Warning Signs	17
Exporting Spectra	78	Lifting Points	50
F			
FCC Rules and Regulations	18		
Flammable Solvents and Samples ...	16		

M		S	
Macros	75	Safety	
Mains Supply Fluctuations.....	15	Electrical	14
Maintenance		General	14
Air Filter	115	Location and Ventilation	16
Cleaning	101	Summary.....	13
Desiccant	102	Use of Flammable Solvents and	
Overview	100	Samples.....	16
Purging	105	Use of Nitrogen.....	16
Source	111	Sample Area Cover	
Windows	113	Removing.....	47
Moving the Spectrometer.....	50	Sampling Accessory	
Lifting Points	50	Changing.....	47
N		Saving Spectra	77
Nitrogen	16	Scanalyze	76
O		Search	69
Optical System		SendTo.....	80
Stability.....	21	Shipping Container	
P		Opening	32
Parts	118	Software	
Optional	118	Component Checks	86
Replacement	119	Exit	98
Upgrades	119	Exporting Spectra	78
Peak Area/Height	71	Help	61
Peak Table.....	67	Humidity Shield.....	88
Power Switch	23	Installation	36
Printing	82	Instrument Install Wizard	46
Purging.....	105	Instrument Settings	83
Gas Regulator Pressure	106, 110	Overview	54
Instrument	108	Power Save	90
Sample Compartment.....	106	Printing	82
Q		Processing Spectra.....	66
Quant.....	71	Quality Checks.....	64
Quantification	71	Reporting	81
Equations	74	Saving Spectra.....	77
Peak Area/Height.....	71	Scanning Samples.....	62
Quant	71	Send To	80
R		Spectrum Workspace	58
Ready Checks	92	Starting Spectrum	55
Reporting	81	Source	
Requirements	30	Replacing	111
Electrical	30	Specifications	31
Environment.....	30	U	
Resolution	84	Unpacking.....	32
R		W	
Ready Checks	92	WEEE Directive	125
Reporting	81	Windows	
Requirements	30	Installing/Replacing.....	113
Electrical	30	Windows Start Menu	55
Environment.....	30		
Resolution	84		



DISTRIBUTED BY:

Sedulitas

PEOPLE | PASSION | PRECISION

info@sedulitas.co.za +27 (0)82 551 4001
www.sedulitas.co.za