# OMNIC v8.3 Release Notes September 2011 Update

About OMNIC	15
DMNIC v8.3	15
New Features	15
Windows 7, 64 bit support	15
Resolved Issues	15
OMNIC	15
IR200, Corrected problems with background handling	15
iS5, Corrected occasional iD5 accessory test errors	
iS10, Corrected error in the iTR experiment file affecting spectral interpretation	
Revised installation process to eliminate compatibility problems with McAfee Update Agent.	15
Known Issues	16
OMNIC	16
ACD Structures optional software is no longer available	
	10
DMNIC v8.2	16
New Features	16
System Performance Verification (SPV)	16
Nicolet iS5	
Antaris IGS II	
Windows 7 support	
JCAMP Multifile read and write	
Spectra signatures in Reports	
SST – Support for new GaGe card	
Windows 7 –Setting up an automated performance verification	
Resolved Issues	
OMNIC	
Print button is disabled in search result window when using OMNIC DS	
Added two types to Options parameter XAxisMode	
Combining Large Spectral Groups in OMNIC 8 Fails	
iS10 filter wheel remains in beampath after ValPro run	
Collect sample error on 4th scan Nexus benches with new sources show Source Current	
Software crash when multiple spectra are opened	
Cannot change X axis scale to nanometers via DDE command	
Search	
Search Libraries and Groups error	
Series	
No Prompt for Temperature or Pressure when required by quant method	
Unable to import TGA data with negative values	
Cannot create correlation map profile on reprocessed rapid scan data	
TQ Gas Quant method corruption leads to erroneous Series CNC file	

Macros Basic Macros Basic delay does not keep accurate time Macros Basic cannot open more than one file	19
OMNIC DS Data Security Remove Run OMNIC Only Digital signature not shown on reports	19
SST and TRS	19
OMNIC v8.1 SP1	19
Resolved Issues Experiment files were getting saved with the Validation Wheel set to the NG11 position after a V run Sample collection crashes when monitoring ValPro methods for both the main FTIR instrument a or more accessories using SPV, the collect background before sample option is selected in Exper Setup and you are using the 21CRF11 option.	ValPro 19 nd one riment
OMNIC v8.1	20
New Features QCheck printout now indicates High Sensitivity option	
Resolved Issues	20
OMNIC OMNIC version 5.1a quant methods now quantify correctly using OMNIC 8.0 SP1 Validation wheel positioning Macros Pro programs Translation Updates:	20 20 20
OMNIC v8.0	20
New Features QCheck System Performance Verification (SPV) OMNIC Specta Nicolet iS10 ThermoIQ Windows Vista support	20 20 21 21 21
Resolved Issues	
OMNIC         Correction Settings in Experiment Setup are offset.         Apodization and Phase Correction Settings in Spectral header of imported JCAMP files may be incorrect.         Saving spectra with blank regions to CSV loses X value information.         Bruker <sup>®</sup> files in %Transmittance scaled incorrectly.         OMNIC32.ini file in Windows directory no longer used         Report notebooks become corrupted when too many reports are added	21 21 21 21 21
OMNIC no longer allows spectra from commercial libraries to be saved	
Series Crash when reopening Rapid Scan series files Sampling Information data and time incorrect for Series data	22
Known Issues	22

OMNIC	22
Tabbing in Options and Experiment Setup does not move between controls	22
960 spectrometer help is not provided	22
Uninstalling ValPro causes new SPV features of OMNIC to display errors	23
Macros Pro	23
Macros Pro Macro Panel is no longer included with Macros\Pro	
Wacio Fallei is no longer included with Wacios/Fio	23
Series	
TA Instruments TGA file not being read using OMNIC Open TGA Data File command	
Series 3-D display only shows in black and white	
TA Instruments TGA file not being read using OMNIC Open TGA Data File command	23
OMNIC DS	23
"Run only OMNIC" feature not supported in Windows Vista	
Screen Saver setting from Thermo Security Administrator not supported in Windows Vista	
Screen baver setting from Thermo Security Administrator not supported in Windows Vista	·····2-T
OMNIC v7.4.1	24
Resolved Issues	24
International (Non-English) Installation	24
OMNIC v7.4	24
	2.4
New Features	
Branding changes	
Help Format Change	
Experiment Filename added to list of experiments	
Automatic Atmospheric Suppression improvements	
Limit on zero fill options with high resolution data Additional Jasco file types now recognized	
Resolved Issues	25
OMNIC	25
Report Notebook spectra all shown in red	
Autosave Base Names	
Incorrect error message when saving to full disk	
Interferograms now attached to reprocessed spectra	
Saving data using filenames that include Kanji characters fail	
Derivative command fails from macro if system is language is Japanese	
QC Compare results not available in Macros Basic	
Library Converter now allows output to be put in same directory as input	
Data from some GRAMS format libraries scaled incorrectly by Library Converter	
Data that cross zero on X Axis may crash Find Peaks	26
Paste operation fails on newly created window	26
Autosave sequence number does not always increment from a macro	
Message displayed indicating intermediate collect results would not be displayed	26
Bench and Diagnostic Tabs of Experiment Setup don't center peak	
File Open dialog locks up opening some Mattson files	
Pasting Search results into Log file gives garbled RTF	
Floating-Point overflow when expanding interferogram display in Experiment Setup	
Raman menu shown twice	
Collect Sample with region selected stops update	27
Known Issues	
OMNIC	
Uninstalling OMNIC 7.x on a system that was upgraded from OMNIC 6.1a	27

Tabbing in Options and Experiment Setup does not move between controls	27
Macros Pro	27
Macro Panel is no longer included with Macros\Pro	
Series	28
TA Instruments TGA file not being read using OMNIC Open TGA Data File command	
Series 3D display only shows in black and white	
MNIC v7.3 Service Pack 1 (SP1)	28
New Features	
Change to version numbers shown in About box	
Support of the Nicolet 8700 (USB version)	
New correlation options avoid shifting first scan of collect	
Resolved Issues	29
OMNIC	29
Smart Accessories not recognized in some circumstances on Nicolet 380 and x700	29
Nicolet 6700 with Dual Channel option does not collect correctly	
Spectral Header information not correctly extracted from user libraries	
Check Desiccant button not available for Nicolet 380 systems	
Align results in flat line interferogram on 460 and ECO 1000	
Polarizer wheel does not move to zero on a Nicolet 8700	
Company Logo change on EZ OMNIC Splash Screen Find Peaks locks up if spectrum X Axis crosses zero	
Macros Basic Macros Basic problems with comma for decimal point	
Some Macros saved in Chinese cannot be reopened	
•	
Series	
Incorrect date/time shown for Rapid Scan data Rapid Scan for 380 uses wrong Settle time	
Using more than three Quant components in a Series run causes problems	
Series window can now be closed from DDE without prompt to save data	
GC temperatures not sent to instrument when changed in Experiment Setup	
Rapid Scan on 8700 PCI misses scans	
Timing of Series collect with external trigger starts before trigger	
Generation of CNC file for profiles created post analysis	
Known Issues	31
OMNIC	
Uninstalling OMNIC 7.x on a system that was upgraded from OMNIC 6.1a	
Tabbing in Options and Experiment Setup does not move between controls	
Macros Pro	32
Macro Panel is no longer included with Macros\Pro	
Series	32
TA Instruments TGA file not being read using OMNIC Open TGA Data File command	32
OMNIC DS Data Security	
Require Signature When Saving Spectrum and OMNIC for Almega	32
MNIC v7.3	32
New Features	27
1 YC WY I СШИГСЭ	

OMNIC	32
Conversion of PerkinElmer, Bruker, GRAMS/Spectral ID & Sadtler SearchMaster libraries	
New interactive Kramers-Kronig correction	
Ability to set the parameters for automatic baseline	
Added the ability to apply a linearization method to photoacoustic data	
Titles of the spectra in the search list are now displayed in overlay mode	
Added the ability to include the name of a notebook in a report	33
Clipboard button added to Search Results window	
Tabular data written to Clipboard as RTF	
OMNIC can control Antaris model spectrometers	34
Series	34
Series data collect has been updated	
Series supports FT-Raman and dispersive Raman spectrometers	
Opening and saving series data files has been updated	
Series 3D display features has been enhanced and updated	
Enhanced display options for series data profiles	
Processing of Series files is integrated into OMNIC menus	
Searching of a spectrum from a series data collect	
Saving of intermediate data during a series collect	
Ability to use basis vectors from a saved file	
Interferograms can be saved during a series collection	
Split series supports long file names	
Series features supported by Thermo Security Administration	
EZ OMNIC	
Automatic Atmospheric Suppression now supported in EZ OMNIC	
Advanced ATR now available	
EZ OMNIC now supported by DS and Thermo Security Administration	
Print/Preview Report is available	
Software IQ	36
New application provided with OMNIC DS to verify software installation	36
Resolved Issues	36
OMNIC	
Selected spectra not retained when added to a notebook	
Title of a newly created notebook was incorrect when the notebook was viewed	
Displayed data collection information is not added to the report in a notebook	
The base file name for autosave has been expanded to 32 characters	
The down arrow control for viewing the list of spectra disappeared after hiding a spectrum	
Cannot not label peaks or pick peaks if spectra are in wavelength	
Could not print out entire list of QC Compare libraries if greater than one page	
Auto file naming spectra in a macro could give odd file names	
Selecting a new initial library directory in Options was not seen in Library Setup	
Y-axis annotations are fixed at 3 decimal points	
If region search is used, the regions are not displayed in the Search Result window	
Copying and pasting an OMNIC window with a selected area does not display the region correctly	
MS Word	
The options in the bench tab of experiment setup are not properly updated if a Smart Accessory is	
changed	
If match settings is used in Library Manager to collect a spectrum, it does not follow the options s	
number of background scans	
Autoblanking regions can cause Advanced Diagnostics tests to fail	
Spectral range for the diamond Smart Orbit gives improper out-of-range warnings	
Default report template not set at install	38

When the information produced with the region tool is removed after the region is drawn Messages of inappropriate parameters in the experiment file do not indicate which parameter was incorrect	
OMNIC may crash when reprocessing libraries created with OMNIC 6	
EZ OMNIC	
Selecting an *.spa file in Windows Explorer and double-clicking does not launch EZ OMNIC	
A default experiment file is not selected during the installation	
Val-Q <sup>TM</sup> autotester will not run with EZ OMNIC	39
Peak Resolve	39
Wrong peak may be highlighted when editing peak table	39
Thermo Security Administration	10
Access to adding a library spectrum to a window is not totally controlled with Thermo Security	.40
Administration	40
Report templates could be overwritten when prevent overwriting files was enabled in Thermo Security	
Administration	
Thermo Security Administration allows any valid user to log in	
Thermo Security Administration fails to add domain user to policy groups	
Unable to sign files a second time if prevent overwriting is enabled	
Additional Analyze menus items are being disabled	
Additional Analyze monus tems are being disubled	
OMNIC v7.2a	40
Resolved Issues	.40
OMNIC	41
Font used for axis on printed reports very small or very large	41
Bitmaps that overlap other fields of report fail to print	41
Printing to non-Default printer may use incorrect font size	
Username provided to ValPro not correct	
Access Violation when collecting data from a Macros\Basic macro	41
Y Axis label incorrect when importing some Perkin-Elmer files	
Access Violation when setting up Atmospheric Correction	
Atmospheric Correction controls disabled in EzOMNIC	42
OMNIC DS	
Save Group (.SPG) does not generate an event log record	42
OMNIC v7.2	42
New Features	42
OMNIC	42
ValPro compatibility	
OMNIC DS	
Individual control of ancillary OMNIC programs launched from OMNIC	
MACROS PRO	43
Environment variables can be used in arguments	
New "Locked" mode available for the OmnicMode command	
New "Overscale" command for scaling and aligning spectra	
Resolved Issues	.45
OMNIC	43
Correct diagnostic information displayed in OMNIC for a Nicolet 380 instrument	44
Automatic atmospheric suppression available with Nicolet 380 instrument	

Single-sided interferogram available with Nicolet 380 instrument Verify smart accessory available with Nicolet 380 instrument	44
Saving spectra from Search results window	
Search and QC Compare from Macros Basic do not require user action to proceed	
Report fields not displayed when editing templates fixed	
Autosave filename in title dropping last character fixed	
Spectra not scaled properly when read from GRAMS multifiles	
Save Range changed when it should not have in Experiment Setup	
Recommended Save Range not including Window Material when Bench tab first displayed	
Find Peaks deletes peak labels outside of the region it is applied to	
Preview Collect controls appear in collect window after a resize or change focus	
DDE Initiate messages no longer destroy global atoms	
Correct Velocities now displayed for Nicolet 380	
Nicolet 380 does not work with the Centaurus microscope	
Cannot set Low pass filter on Nicolet 8700	
External trigger with a Nicolet Series instrument only works the first time	46
MACROS PRO	46
Export command displays save dialog when it should not	
OMNIC v7.1a	46
Resolved Issues	46
OMNIC	46
OMNIC unstable after leaving Bench tab of Experiment Setup	47
Detector changes when Sample Compartment list is viewed	
OMNIC v7.1	
New Features	47
New Features	
OMNIC	47
OMNIC Peak Resolve	47 47
OMNIC Peak Resolve Faster Control of Nicolet Series Instruments	47 47 47
OMNIC Peak Resolve. Faster Control of Nicolet Series Instruments New default configuration file	47 47 47 47
OMNIC Peak Resolve Faster Control of Nicolet Series Instruments New default configuration file Support added to Nicolet Series and Nexus drivers for Continuum XL	47 47 47 47 47
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.	47 47 47 47 47 48
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.	47 47 47 47 47 48 48
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.	47 47 47 47 47 48 48
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.	47 47 47 47 47 48 48 48
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation	47 47 47 47 48 48 48 48 48
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.	47 47 47 47 48 48 48 48 48 48 48
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.	47 47 47 47 48 48 48 48 48 48 48 48
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.	47 47 47 47 48 48 48 48 48 48 48 48 48 48 48
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.	47 47 47 47 48 48 48 48 48 48 48 48 48 48 49 49 49
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.	47 47 47 47 48 48 48 48 48 48 48 48 48 49 49 49 49
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation.         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.	$\begin{array}{c}47\\47\\47\\48\\48\\48\\48\\48\\48\\48\\48\\48\\49\\49\\49\\49\\49\\49\\49\\49\\49$
OMNIC	47 47 47 47 47 48 49
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation.         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.	47 47 47 47 47 48 49
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation.         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.         Kinetics.         New Array menu items.	$\begin{array}{c}47\\47\\47\\47\\48\\48\\48\\48\\48\\48\\48\\48\\48\\49\\49\\49\\49\\49\\49\\49\\49\\49\\49\\50\end{array}$
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.         Kinetics.         New Array menu items.	$\begin{array}{c}47\\47\\47\\47\\48\\48\\48\\48\\48\\48\\48\\49\\49\\49\\49\\49\\49\\49\\50\\50\end{array}$
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.         Kinetics.         New Array menu items.	$\begin{array}{c}47\\47\\47\\47\\48\\48\\48\\48\\48\\48\\48\\49\\49\\49\\49\\49\\49\\50\\50\\50\\50\\ \end{array}$
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.         Kinetics.         New Array menu items.         MACROS PRO         Replaceable collect prompts.         Interferogram peak level readable from Nicolet Series instruments.	$\begin{array}{c}47\\47\\47\\47\\48\\48\\48\\48\\48\\48\\48\\49\\49\\49\\49\\49\\49\\50\\5$
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.         Kinetics.         New Array menu items.         MACROS PRO         Replaceable collect prompts.         Interferogram peak level readable from Nicolet Series instruments.         Environment variables supported in run commands.	$\begin{array}{c}47\\47\\47\\47\\48\\48\\48\\48\\48\\48\\48\\49\\49\\49\\49\\49\\49\\49\\50\\$
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.         Kinetics.         New Array menu items.         MACROS PRO         Replaceable collect prompts.         Interferogram peak level readable from Nicolet Series instruments.         Environment variables supported in run commands.         OMNIC DS	$\begin{array}{c}47\\47\\47\\47\\48\\48\\48\\48\\48\\48\\48\\49\\49\\49\\49\\49\\49\\49\\49\\50\\50\\50\\50\\50\\50\\51\end{array}$
OMNIC         Peak Resolve.         Faster Control of Nicolet Series Instruments.         New default configuration file.         Support added to Nicolet Series and Nexus drivers for Continuum XL.         Environment variables now allowed in Menu and Toolbar paths.         JCAMP-DX Enhancements.         More pre-peak data points used for Raman collect above 4 cm-1 resolution.         Array Automation         Added ability to skip wells.         Improvements to the Array: Open Data Set window.         Change well selection using arrow keys.         Quant report allows All choice.         Region controls provided for specifying correlation region.         Peak height ratio and Peak area ratio metrics available in reprocess.         Kinetics.         New Array menu items.         MACROS PRO         Replaceable collect prompts.         Interferogram peak level readable from Nicolet Series instruments.         Environment variables supported in run commands.	$\begin{array}{c}47\\47\\47\\47\\48\\48\\48\\48\\48\\48\\48\\49\\49\\49\\49\\49\\49\\50\\50\\50\\50\\50\\51\\5$

Administrator program more easily adds or removes access control entries for all access control	
functions	
Support for signing protect group files (.spg).	
Sign multiple files with a single authentication prompt	
Sign the selected spectra without using a file navigation dialog.	
Atlµs v7.1 Support for Nicolet Series Bench	
Resolved Issues	
OMNIC	
Company Name change	
Current Tool changed after running a Macros Basic macro	
Spectrum title corrupted by Automatic Baseline Correct.	
Asterisk appended to spectrum filename	
X Axis not drawn at start of data collect	
X Axis always in decreasing order in Collect Window	
X Axis limits changed at end of Raman collect	
Multiple copies of Spectral Group files sent with Mail Spectra	
Collection and Processing Window garbled after closing spectral window	
Interferogram peak not in display window of Experiment Setup	
Overlay feature of Search results does not work when decimal point is a comma	
Use Fixed Scale during data collect not applied to interferogram collects	
Buttons at bottom of Experiment Setup and Options cutoff when large fonts are used	
Dialog font intermittently incorrect	
Extended Search text fields too short	
Green check appears before bench communications established	
Loading an old (pre 7.0) experiment file does not reset new fields	
Problems with beamsplitter recognition on Nicolet Series instruments	54
OMNIC DS	54
Editing annotation in the Annotation Information dialog corrupts signature status display	
Known Issues	54
Tabbing in Options and Experiment Setup does not move between controls	
Inserting a smart accessory during a data collect.	
MNIC v7.0	5
New Features	5
OMNIC	5
Anti-collision for annotations in Find Peaks.	5
Support for Nicolet Series instruments	5
Grid of controls used on Bench tab of Experiment Setup.	
Freeze button on Bench and Diagnostic tabs of Experiment Setup	
New Configure tab of Experiment Setup	
X Limits of live display persist in Experiment Setup.	5
Background scans optionally set separate from Sample scans.	
Background scans optionally set separate from Sample scans.	-
Option to set Y-Limits for use during collect.	S
Option to set Y-Limits for use during collect.	
Option to set Y-Limits for use during collect Auto-blank regions during data collect	5
Option to set Y-Limits for use during collect. Auto-blank regions during data collect. Marco assigned to front panel button on instrument.	5 5
Option to set Y-Limits for use during collect. Auto-blank regions during data collect. Marco assigned to front panel button on instrument. Improved peak annotations.	5 5
Option to set Y-Limits for use during collect. Auto-blank regions during data collect. Marco assigned to front panel button on instrument. Improved peak annotations. Annotations viewable as a table.	50 50 50
Option to set Y-Limits for use during collect. Auto-blank regions during data collect. Marco assigned to front panel button on instrument. Improved peak annotations. Annotations viewable as a table. Mail Spectra.	5 5 5
Option to set Y-Limits for use during collect. Auto-blank regions during data collect. Marco assigned to front panel button on instrument. Improved peak annotations. Annotations viewable as a table.	5 5 5 5 5

Additional techniques supported for Derivative.	57
Overlay spectra in Search Results window	
Multifile .SPC file read	
New look for tabbed dialogs	
Saving spectra from Spectral Group files now defaults to saving as individual files	
Floating-point exceptions now handled more gracefully	58
OMNIC DS	58
Administrator program translated	
Warning at OMNIC start for invalid directory policies	
SST and TRS	58
Synch Hold Addition to SST	
Resolved Issues	
<i>OMNIC</i>	
Collect time-out when set to ssp1 @ .125 cm-1 resolution with PCI card	
Problems showing data in increasing X order fixed.	
File types recorded separately for Open and Delete file dialogs.	
Filename now shows when bitmap pasted into external program.	
Mpanel32.exe no longer installed	
Collection and Bench parameters saved in new user libraries for each spectrum.	
Spectrum filename can be displayed in Search window	
Improved parsing of OMNIC command line	
Changes made to spectra extracted from report do not affect report display	59
OMNIC DS	60
Saving data to protected directories works as installed.	
Problems signing files after password change on Windows XP fixed	
Print feature of Search window now uses printing policy correctly.	
Spectra extracted from library can now be printed regardless of printing policy	
Windows key no long gives access to explorer features in open/save dialogs.	
Event log entries now made for file deletions for GAML files.	60
OMNIC v6.2	60
New Features	60
OMNIC	
Read/Write GAML files.	
New Advanced ATR correction.	
Insertion and deletion date now available for library spectra.	
Spectra deleted from user libraries remain visible until the library is compressed	
Display help files in three-pane mode.	
Resizing Open/Save dialogs.	
Remember size of Spectrum information window	
Record old data spacing for Change Data Spacing	
Raman operations generate history records.	
Change Data Spacing history now includes old data spacing	02
OMNIC DS	62
Admin program for configuring user authorization	62
Reasons for Digital Signatures controlled by Admin program	
Event Log for significant events	
Saving data to directories with restricted access	
Sign file gives three chances to enter correct password.	62
SST and TRS	62
New Sample Spacing choices	
Sharang encirco	

Improved multiple-trigger mode	
Resolution selection for step-scan time-resolve	63
Y-axis added to TRSS real-time display	63
Step-Scan Settling time now set with edit control	63
Resolved Issues	63
OMNIC	63
Change the default setting for the Bench and Collect checkboxes to off in the Quant Setup of	
Change how the spectral limits in a new Raman library will be created	
Change to not display an error when a user chooses not to overwrite a signed file	
Fixed a bug that occurred when OMNIC was installed in a path that used multi-byte Japanese	
On a clean install, the default for peak picks will be sorted on Position, not intensity	
Setting access rights to temporary directory	64
Turn off display of signature information in reports.	64
Spectra from signed .spa files appear modified when loaded	64
Change to allow up to 10000 series files in sequence rather then 100.	64
Cleanup drawing flaws in skinned dialogs.	64
Fixed a bug that would disable the spectrometer tour by mistake in some cases.	64
MRU list saved on a per-user basis.	
OMNIC sub-installers have been changed to use Microsoft Installer.	65
Spikes in files converted from Perkin Elmer format fixed.	
Undo Scale must be done twice	65
Raman Instrument correct works with a reference file	65
Options changes recognized in Find Peaks window	65
Drawing shaded regions on 32 bit depth ATI cards changed.	65
Additional message generated if file signing canceled	65
References to Thermo web site changed.	
Crash when invalid gain read from a file	66
More scans button on collect window disabled for Mattson.	66
Failure to overwrite read-only configuration files now reported	66
Failure of Change data spacing now reported.	66
Hourglass cursor now shown during Other Conversions.	
Digital Signature status not shown properly for Almega spectra	66
Text drawing bug in collect status window fixed	
Spectra filename lost after an undo operation fixed	66
Crash when adding very long annotation fixed	66
Remove DC offset from interferograms read from Mattson files	67
Normalize Scale command failed when performed twice.	67
Change to the default value in Quant setup.	67
Raman data added to library had poorly registered X-axis values.	
Initial directory for Configuration files is now the same as parameter files	
GC-FTIR External trigger feature fixed	
SST and TRS	67
Display of Channel B/A ratio in PEM setup dialog	
Collect time-out problem in step-scan dialogs.	
Phase Analysis dialog.	
SST menu item names.	
OMNIC v6.1a	68
Resolved Issues	
OMNIC	
The new GMT time zone information in the Data Display Information section of the Spectra displayed improperly when on the positive side of the grand meridian.	

Changed the Spectrometer Tour routine to not check the CDROM drive for the tour Rapid scan collects stalled on Windows NT 4.0 systems	
Intermittent driver problem could result in a system lockup during data collect	
InterpretIR+	
InterpretIR+ did not install from the Update CD	68
Val-Q	68
Some Autotest results report failures when run under some foreign languages.	
Autotest report four failures when run on a system that does not have the DS option installed	
View Stage	69
Cannot view data during data collection.	
Almega	69
Photobleaching not operating properly	
Slit selection changing when switching tabs.	
Autogain limits and trigger intervals.	69
OMNIC v6.1	70
New Features	70
Display limits when viewing data in nanometers	
When copying a report to the clipboard, the report is placed in the clipboard as a bitmap as well a	s a
metafile	
Added new 'GetBenchName' DDE routine. It gets the bench name and puts it into result current.	
Added new Delay DDE command. It can be used in a macro to delay for a specified number of sec	
Enabled the "Other Conversions" menu command in the Process menu of EZ OMNIC.	
Improved Issues	71
Substantially decreased the amount of time to start OMNIC for Nexus and Avatar series spectrom	eters
Substantially decreased the amount of time to start OMNIC when using the Digital Signature (DS	
option on a computer that is not physically connected to a network.	
Added capability to capture the user name with every modification that is recorded in Collection a	
Processing Information	
If a digitally signed spectrum is modified but not saved, the display of that spectrum would chang	e to
"Spectrum not signed". This is not correct as the file saved on disk still has a valid signature	
Record the signing of a spectral file in the Collection and Processing Information	
Added ability to have an NTFS folder with RWX permission (no delete) and allow spectral file sa	
Changed atmospheric suppression feature so that during data collection, the suppression is only	12
Changed atmospheric suppression feature so that during data collection, the suppression is only performed if the result is improved when compared to the result from the unsuppressed spectra	72

Enhanced axis routines to improve annotation capabilities when spectra are displayed in waveleng	
Add in capability to call DDE annotate command with only 2 arguments, if no text is specified use	
or x&y position for the annotation text	
Add capability to display information from Almega data files such as laser wavelength and grating	
the Collection and Processing Information when viewed in workstation OMNIC	
Changed resource text "The spectra have different Y-axis units." to "The spectra have different ax	
units." This text was used to refer to different X and different Y-axis units.	
Added cue card help for various tool palettes within OMNIC.	
Improved COM interface to DDE commands to insert '[' characters if needed and to properly wai	t for
command completion before returning from the command for asynchronous commands	
Added support to add COM objects to OMNIC functionality at run time	73
Resolved Issues	73
OMNIC	71
Request to store the name and path of the background file in the Collection and Processing Information	
Request to store the name and pair of the background me in the concerton and rocessing morning	
In the Collection and Processing Information, the data collection error information is displayed on	
screen but not printed.	
If a spectrum was extracted from a notebook, the collection time that appeared in the Collection as	
Processing Information was that of the last spectra from the lab notebook	
Changed text from "Signature could not be verified" to "Signature could not be verified because the	
necessary software or operating system is not present." This occurs on Win98 or when DS not	
purchased.	74
OMNIC sign read-only files. Put in test for read-only files before attempting to sign them. Now put	
an error message when they are read-only	
Performing a search of a digitally signed spectrum changed the status in the display of that spectru	
"Spectrum not signed."	74
Unable to configure a custom detector on the right hand side of the spectrometer.	
Spectral range for XT-KBr beamsplitter and DTGS TE cooled is not correct.	
Changed to allow reset bench at start of Raman data collection.	
The sample compartment validation wheel for the Avatar does not work with OMNIC 6	
If a Mattson spectrometer had a communication failure when in Experiment Setup, the user had to	
and then re-open the Experiment Setup dialog to resume communications.	
Changed OMNIC to not require a default.cfg file on startup. It creates one if needed now	
Fixed tiny memory leak when a new background is collected. Only a problem for repeated backgr	
collects over days.	
Modify Reprocess to account for the fact that an atmospheric suppression might be done on a spec	ctrum
with SSP equal to one	75
The Save Group command does not let the user save to a network folder with an UNC path	75
OMNIC .SPA files are not associated with the OMNIC application	75
OMNIC could not read in some older PC-IR data files	
If you save a spectrum as a CSV file, the entire spectrum is being saved to the file instead of only	
displayed region	
Mattson files other than .abs are not saved properly.	
Modified JCAMP-DX to always write out LONGDATE for Y2K compliancy. Additionally, a small	
change to continue writing out JCAMP-DX the old way for dates less than 2000. That is 10/04/97	
write out dates new 4 digit way when greater than 1999	
If the spectra were being displayed in wavelength, the only option allowed in for an X-axis format i	
Display Options was Normal.	
If the Sampling Information, enabled through the Display Setup dialog in the View menu, did not fi	it one
a single line, the text would not print. Need to correctly determine width of printable area for text	
wrapping. Fixed issues where if text enabled through Display Options wraps, it would not print	
Under Display Setup, choosing overlaid titles and displaying sampling information caused the tex	
overlap	/6

The spectral title will not print if an annotation's starting point was near 2500 cm-1. Also, long spectral titles will not print if the title cannot fit on a single line
If one copies and pastes an OMNIC window into a program such as MS Word or PowerPoint, it is
copied with the New Window axis limits instead of the displayed values
systems
Enabled cue-card help for Copy and Sign buttons in the report feature
If the Roll & Zoom command is chosen, pressing F1 for help brings up the help topic for saving
configurations
Help menu items are not be displayed according to the Edit Menu configuration
If "Text Only" is selected for the OMNIC Toolbar, the toolbar button separator and the button frame do
not appear
The Command Text label in the Add Item Dialog in Edit Menu is not changing consistently with the Item Type
The colon after "Experiment" for the experiment drop down control on the main OMNIC window is
hidden
Fixed issue when if the computer's display mode was set to 256 or less colors, the subtract auto Y check box could not be checked
Update look of "Change data spacing" dialog to match new OMNIC 6 blue textured look
Basic Macros and Macros Pro       78         Same Desig Macros model and bitter it with a the mark from the ONDUC to the operation of the Control of t
Some Basic Macros would crash intermittently when run from the OMNIC toolbar
command is not invoked from DDE
Modified "Statistical Spectra" to not show New Window prompt if command invoked from DDE79
nterpretIR+
InterpretIR+ does not automatically import the active spectrum from OMNIC when launched79
Atlµs, µView™ (Microview) and View Stage
Atlµs, µView™ (Microview) and View Stage79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to set the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79
Atµs, µView™ (Microview) and View Stage
Atlµs, µView <sup>TM</sup> (Microview) and View Stage       79         Expanded support to allow Atlµs maps to contain up to 50,000 spectra.       79         Request to save the image size when Atlµs (or Microview) is closed so that the program automatically recalls the values for the user.       79         Request to set the number of background and sample scans to different values in Map Setup within Atlµs.       79         Atlµs does not autofocus for each video frame when collecting a mosaic with a map       79         Microview opens in a small window after installation.       79         The ruler in the navigation pane of Atlµs cannot be moved with the mouse.       79         Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly.       80         With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and
Atlµs, µView™ (Microview) and View Stage79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to set the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly.80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80
Atlµs, µView <sup>TM</sup> (Microview) and View Stage79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to set the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly.80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80View Stage users cannot access Atlµs or µView (Microview) correctly. Provide a calibration file for the
Atlµs, µView™ (Microview) and View Stage79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to set the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly.80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80View Stage users cannot access Atlµs or µView (Microview) correctly. Provide a calibration file for the View Stage so that users can then use Atlµs or µView.80
Atlµs, µView™ (Microview) and View Stage
Atlµs, µView™ (Microview) and View Stage.79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to save the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly.80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80View Stage users cannot access Atlµs or µView (Microview) correctly. Provide a calibration file for the View Stage so that users can then use Atlµs or µView.80Val-Q80Spectral group collected in Val-Q could not be saved to a network drive.80
Atlµs, µView™ (Microview) and View Stage.79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to save the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80View Stage users cannot access Atlµs or µView (Microview) correctly. Provide a calibration file for the View Stage so that users can then use Atlµs or µView.80Val-Q8080OMNIC experiment parameters are not being restored to previous settings when Val-Q closes.80
Atlµs, µView™ (Microview) and View Stage79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to save the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly.80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80View Stage users cannot access Atlµs or µView (Microview) correctly. Provide a calibration file for the View Stage so that users can then use Atlµs or µView.80Val-Q80Spectral group collected in Val-Q could not be saved to a network drive.80Series80
Atlµs, µView™ (Microview) and View Stage79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to save the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly.80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80View Stage users cannot access Atlµs or µView (Microview) correctly. Provide a calibration file for the View Stage so that users can then use Atlµs or µView.80Val-Q80Spectral group collected in Val-Q could not be saved to a network drive.80Series80Fixed bug that prevented import of TGA files into series.80
Atlµs, µView™ (Microview) and View Stage79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to save the number of background and sample scans to different values in Map Setup within79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80View Stage users cannot access Atlµs or µView (Microview) correctly. Provide a calibration file for the View Stage so that users can then use Atlµs or µView.80Val-Q80Spectral group collected in Val-Q could not be saved to a network drive.80Series80Fixed bug that prevented import of TGA files into series.80Series and Atlµs progress bar now painted with new OMNIC 6 blue textured dialog style colors80Series and Atlµs progress bar now painted with new OMNIC 6 blue textured dialog style colors80
Atlµs, µView™ (Microview) and View Stage79Expanded support to allow Atlµs maps to contain up to 50,000 spectra.79Request to save the image size when Atlµs (or Microview) is closed so that the program automatically79Request to save the number of background and sample scans to different values in Map Setup within79Atlµs.79Atlµs does not autofocus for each video frame when collecting a mosaic with a map79Microview opens in a small window after installation.79The ruler in the navigation pane of Atlµs cannot be moved with the mouse.79Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly.80With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.80View Stage users cannot access Atlµs or µView (Microview) correctly. Provide a calibration file for the View Stage so that users can then use Atlµs or µView.80Val-Q80Spectral group collected in Val-Q could not be saved to a network drive.80Series80Fixed bug that prevented import of TGA files into series.80

Problems?	84
OMNIC Installation Directories	84
Known Issues IR Spectral Interpretation will not display the functional group information (accessed by clicki eyeglasses) if Library Manager is open	ng on the
SST and TRS	
contains "(H)", if at low intensity it contains "(L)".	83
Added code to bin-in-memory collects to check for CCD traps Modified DDE commands so that calibrations can be run from macro (no finish dialog) and un collects finish correctly Spectrograph alignment tab changed so that if LED is at high intensity during pinhole align, N	83 n-invoked 83
initialized to checked. Turn both lasers On/Off option on Advanced tab does not stay selected. Disable this option if laser installed. Fixed bug that occasionally introduced a blank data point in spliced spectra.	
Added initialization code so that the correct grating is selected when entering the Bench or Al This also fixes bug, which caused occasional blank spectral range text boxes when selecting 5 Res grating Automatic data spacing option on Advanced tab not always selected by default. Changed so it	ign tab. 532 Low 83
Require a laser normalize for atypical laser type spectrometers. Add methods to calculate the resolution information for atypical lasers. Changed startup code to detect when bench power is off and prevent showing multiple camera	
Laser calibration improvements. Almega Installation Issues. Do laser accordian before Set_fold_limits to get desired range.	
If the focus button is clicked rapidly with a 50x objective, the focus motors may not be able to object back in focus. Manual refocusing required The signal is not changing during autoalign if option 3, align laser to pinhole, is selected Wavelength calibration. Improved algorithms to make calibration more robust	
Added Photobleach time to collect tab; removed estimated resolution as it is on the Bench tab. Added partial wavelength calibration feature. This lets the user select a subset of spectral rang calibrate if they don't want to take the time to calibrate all ranges. Changed the alignment procedure to start at the center and spiral out rather than raster a rectar Coarse adjustment needs a finer scale.	
If one uses the same peak and baseline values for the numerator and denominator in Profile se "Peak height ratio of two peaks", the Y readout was displayed as "1.#QQ"	etup for 81
potential file (more than supported)	
resultant file would be larger than is supported. Also file creation to return 0 if too many spect	tra in

# About This Document

This document contains information about the OMNIC<sup>™</sup> version 8.3, 8.2, 8.1 SP1, 8.1, 8.0 SP1, 8.0, 7.4.1, 7.4, 7.3 Service Pack 1 (SP1), 7.3, 7.2a, 7.2, 7.1a, 7.1, 7.0, 6.2, 6.1a and version 6.1 software suite, including new features, questions from our users and known issues.

# About OMNIC

Thermo Scientific OMNIC software is a full-featured package that provides all the tools necessary for Fourier transform infrared (FT-IR) and Raman analysis. OMNIC software allows you to quickly and easily collect, process, analyze and manage your FT-IR or Raman data in a graphical environment that is customizable and easy to learn. It is the common platform used by all Thermo Scientific laboratory spectrometers and is the heart of the Thermo Scientific Smart System approach to spectroscopy, providing a critical level of integration between software, spectrometer and sampling accessory.

OMNIC 8.3 is a spectroscopy software package that runs in Windows<sup>®</sup> XP Professional, Windows Vista<sup>®</sup> Business, Windows 7 Professional 32-bit, or Windows 7 Professional 64-bit. Consult the computer requirements document for additional requirements for individual hardware or software components. Earlier versions of OMNIC could be used on other versions of Windows.

# OMNIC v8.3

# **New Features**

# Windows 7, 64 bit support

**Description**: OMNIC 8.3 is now supported on systems with Windows 7 Professional edition, 64 bit version.

# **Resolved Issues**

# OMNIC

# IR200, Corrected problems with background handling

**Description**: Beginning with OMNIC 8.2, the data spacing adjustment for the instrument's diode laser was not applied correctly when the background was measured resulting in invalid background errors.

# iS5, Corrected occasional iD5 accessory test errors

**Description**: Occasionally the automated accessory test, which runs when the iD5 accessory was attached, would initially indicate a failure but always succeed when re-tried.

# iS10, Corrected error in the iTR experiment file affecting spectral interpretation

**Description**: An incorrect value in the iTR experiment file for iS10 prevented the Spectral Interpretation operation from producing the expected result.

# Revised installation process to eliminate compatibility problems with McAfee Update Agent

**Description**: On some systems with McAfee, the McAfee Update Agent would no longer run properly after installation of the OMNIC software.

# Known Issues

# OMNIC

# ACD Structures optional software is no longer available

Description: This package is incompatible with Windows 7 and has been removed.

# OMNIC v8.2

# New Features

# System Performance Verification (SPV)

**Description**: The SPV feature has been enhanced to support the new Nicolet<sup>™</sup> iS<sup>™</sup>5 instrument. A check box has been added to the System Suitability test to do an auto tune at the start of the test.

# Nicolet iS5

**Description**: Added support for the Nicolet iS5 spectrometer. This includes the laser calibration, warm up time when the instrument is first started and a prompt to run PV when the instrument is first used.

# Antaris IGS II

**Description**: Added support for the IGS II spectrometer and data collection in series at high speed.

# How to use 5 Hz, 0.5cm-1 series collect:

Set the following parameters in Experiment setup

On Collect tab set

No. of scans = 4

Resolution = 0.5

Turn off automatic atmospheric suppression

On Bench tab set

Optical velocity = 8.2277

On Advanced tab set

- Zero filling = none
- Sample spacing = 2

On Series tab set

Data collection type = High speed real time

This collects full spectra using the bidirectional collect.

Profiles – If using quant method, do not select "Use quant method from file" as this will prevent creation of the CNC file. Use the main quant setup under Analyze menu.

Select "Gas Cell" and setup the parameters to use default values or read from the gas parameters if hardware available.

A quant method for the reverse scan can be selected by checking the "Use reverse quant" and selecting "Setup Reverse Quant" to choose a quant method developed for the reverse stroke of the bidirectional scan. This is used to enhance the performance of the series collect.

Select the OK button on Experiment setup.

Select Collect Series and run it as described in the documentation.

Setting up a Reverse quant method.

This quant method is used when "Use reverse quant" is selected in Series setup.

Collect background by using the "Collect Background (bidirectional)..." command. This will create a forward and reverse background set which can be saved to disk as an SPG file.

Collect a standard by using the "Collect Sample (bidirectional)..." command. This will collect two spectra, forward and reverse.

Create the TQ quant method as described in the documentation.

Create a second TQ method by copying the completed first method to a new file. Change the standards in this method to be the reverse spectra collected earlier. So that one method is using forward spectra and the other method has the reverse spectra.

# Windows 7 support

**Description**: OMNIC 8.2 is compatible with Windows 7 Professional edition. 64 bit versions of Windows are not supported.

# JCAMP Multifile read and write

Description: Add support for JCAMP MultiFile read and write.

# Spectra signatures in Reports

**Description**: A report field has been added to show the signature of a spectrum in a report.

# SST – Support for new GaGe card

Description: Support for new GaGe Razor 1422 card for TRS

# Windows 7 –Setting up an automated performance verification

**Description**: The steps for setting up an automated performance verification have changed for the Windows 7 operating system. The user documentation should read as follows:

If Performance Verification is available on your system, you can have a verification run automatically at a scheduled time using the internal validation wheel. You use the Task Scheduler wizard in Windows to set up the software for verification.

In Windows 7:

For View By Category: Click Start > Control Panel > System & Security > Administrative Tools > Task Scheduler to launch the Task Scheduler application. For View By Large or Small Icons: Click Start > Control Panel > Administrative Tools > Task Scheduler to launch the Task Scheduler application.

Choose "Create Basic Task" in the Actions panel of the Task Scheduler and then follow the wizard's instructions. Enter a task name and optional description and configure the trigger information as desired. When asked what action you want the task to perform, select Start A Program. Then use the Browse button to locate and select the file named omnic32.exe. This file is typically in C:\Program Files\OMNIC; the specific location depends on where you installed OMNIC.

In the Add Arguments text box enter the following: -C"PerfVerifyTest; Select All; DeleteSelectedSpectra; Exit"

Type this text exactly as it appears above, including the quotation marks, copying the text from here may not work.

When the "Open the Properties Dialog For This Task When I Click Finish" check box appears, select it and then choose Finish. A dialog box appears. Select "Run only

when user is logged on" in the General tab. Set the parameters on the other tabs as desired and then choose OK.

**Note:** Selecting the option to "Run when user is not logged on" on the General tab will not work as expected for launching a PV test.

# **Resolved Issues**

# OMNIC

# Print button is disabled in search result window when using OMNIC DS

**Description**: If the system policy "prevent printing, cutting or copying of unsaved data" is activated the customer is unable to print from the search result window.

# Added two types to Options parameter XAxisMode

**Description**: The types "NanometerXAxis" and "ElectronVoltXAxis" were added to the DDE parameter for the XaxisMode. The settings were available from the Options dialog in Omnic but not from the DDE parameter.

# **Combining Large Spectral Groups in OMNIC 8 Fails**

Description: Unable to combine two large spectral groups into one file on disk.

# iS10 filter wheel remains in beampath after ValPro run

**Description**: The filter wheel did not switch to the open position after the ValPro test was run.

# Collect sample error on 4th scan

**Description**: During a background collection the software crashed when the collect reached the  $4^{th}$  scan.

# Nexus benches with new sources show Source Current

**Description**: After source replacement the sources work but they fail the source current low limit test.

# Software crash when multiple spectra are opened

**Description**: When using OMNIC DS 8.0 and opening multiple spectra OMNIC displays an unexpected error Caution box.

# Cannot change X axis scale to nanometers via DDE command

**Description**: Omnic returns an error when the DDE command is used to set the X axis scale to nanometers.

# Search

# Search Libraries and Groups error

**Description**: When making a library list a group the following error message would appear "The library or path in the group was not found". The error message is confusing.

# Series

# No Prompt for Temperature or Pressure when required by quant method

**Description**: When the TQ quant method required a prompt for temperature or pressure, the series collect would not prompt.

# Unable to import TGA data with negative values

**Description**: Negative values are occasionally used in the TGA data. This prevented importing of the data into the series run.

# Cannot create correlation map profile on reprocessed rapid scan data

**Description**: Rapid scan data set collected and reprocessed to absorbance. When profile run error message "Cannot recalculate reconstructions with interferograms or single beam spectra. Please change the final format"

# TQ Gas Quant method corruption leads to erroneous Series CNC file

**Description**: Using a TQ quant method that reports errors results in a CNC file with zeros for all the quant values and times of zero when a profile is run.

#### **Macros Basic**

#### Macros Basic delay does not keep accurate time

**Description**: When using a macros basic delay task, it does not keep accurate time.

#### Macros Basic cannot open more than one file

**Description**: Macro is setup to open several files, when executed with several files there was an error.

#### **OMNIC DS Data Security**

# **Remove Run OMNIC Only**

**Description**: The system policy "Run OMNIC only" cannot be supported in Windows VISTA or Windows 7.

# Digital signature not shown on reports

Description: The spectrum digital signature was not shown on the spectrum in a report.

SST and TRS

OMNIC v8.1 SP1

#### **Resolved Issues**

# Experiment files were getting saved with the Validation Wheel set to the NG11 position after a ValPro run.

**Description**: In previous versions of the software sometimes experiment files were saved with the Validation Wheel set to the NG11 position after a ValPro<sup>TM</sup> software run which would then leave the wheel in a position other than home which was not acceptable. The only work around was to restart the OMNIC application following a ValPro run. Now the experiment file settings are set properly so that the correct position is stored following a ValPro run. All experiment files that were saved previously will be adjusted at runtime to correct the issue also.

# Sample collection crashes when monitoring ValPro methods for both the main FTIR instrument and one or more accessories using SPV, the collect background before sample option is selected in Experiment Setup and you are using the 21CRF11 option.

**Description:** The software generates an unhandled exception on the 4<sup>th</sup> scan of the sample collection following a successful background collection when certain ValPro methods are monitored in SPV and TSA is being used. When all of these conditions are met a buffer overflow exception was thrown because of a long description being generated. This issue has been addressed and will no longer occur.

# OMNIC v8.1

# New Features

# **QCheck printout now indicates High Sensitivity option**

**Description**: The result window now displays text indicating the High Sensitivity setting used during the processing.

#### **Resolved Issues**

# OMNIC

# OMNIC version 5.1a quant methods now quantify correctly using OMNIC 8.0 SP1

**Description**: Quant methods created with OMNIC version 5.1a now quantify correctly with OMNIC 8.0 SP1 software. They caused an error to occur when used with OMNIC 8.0.

#### Validation wheel positioning

**Description**: Prior to auto-aligning, the validation wheel is reset to the home position.

#### Macros Pro programs

**Description**: Macros Pro programs will not execute without requiring installation of Macros Pro on the system.

#### **Translation Updates:**

**Description**: The translation files have been updated.

#### OMNIC v8.0

# **New Features**

# QCheck

**Description**: The new QCheck feature allows a user to compare a spectrum to an individual reference spectrum or to a set of reference spectra. The analysis is configured with the QCheck Setup command found in the Analyze menu and the analysis is performed using the QCheck command found in the same menu.

# System Performance Verification (SPV)

**Description**: The SPV feature provides an integrated monitor to verify instrument performance, perform "fit for purpose" tests, and inform the user when tests or maintenance have failed or need to be performed. It consists of the Instrument Status monitor, Scheduled Maintenance monitor, System Suitability monitor, Performance Verification monitor, and ValPro<sup>™</sup> monitor (if installed). If any of those items being monitored need to be performed or have failed, the System Status indicator changes from green to yellow or red as appropriate.

# OMNIC Specta

**Description**: Added support for sending the selected spectrum in OMNIC to OMNIC Specta<sup>™</sup> for further analysis. This is accomplished using the Send to OMNIC Specta command in the Analyze menu.

# Nicolet iS10

**Description**: Added support for the Nicolet<sup>™</sup> iS<sup>™</sup>10 spectrometer.

# ThermolQ

**Description**: The ThermolQ utility is now included with OMNIC; previously it was included with OMNIC DS. This utility allows you to verify that the files on your computer match the files specified by the installer.

# Windows Vista support

**Description**: OMNIC 8 is compatible with Windows Vista Business edition. However, there are two features of OMNIC DS that are not supported in Vista. See the known issues for a description of these limitations.

# **Resolved Issues**

# OMNIC

# Correction Settings in Experiment Setup are offset

**Description**: If you select ATR, H20 or CO2 Correction in Experiment Setup, the software actually performs the correction listed one below your selection.

# History: This problem was introduced in OMNIC 7.4.

# Apodization and Phase Correction Settings in Spectral header of imported JCAMP files may be incorrect

**Description**: The JCAMP file format does not define the apodization function or phase correction settings of a spectrum. In previous versions, OMNIC set these values to OMNIC's normal defaults. In OMNIC 8 these values are set to unknown.

# History: This problem was true in all versions of OMNIC that supported JCAMP.

# Saving spectra with blank regions to CSV loses X value information.

**Description**: If you saved a spectrum with a blanked region to a CSV file, the X-axis information was incorrect for the region above the blanked area. This has been fixed.

# History: This problem was true in all versions of OMNIC that supported saving to CSV.

# Bruker® files in %Transmittance scaled incorrectly

**Description**: Files in the Bruker format with data in percent transmittance (%T) were incorrectly scaled from zero to one instead of zero to 100. This has been fixed.

# History: This problem was introduced in OMNIC 7.3.

# OMNIC32.ini file in Windows directory no longer used

**Description**: Users without Administrator privileges are restricted from writing updates to the Windows\OMNIC32.ini file in most Windows environments. OMNIC has changed to writing shared state information to the file OmnicSettings.ini in the OMNIC data directory (usually

C:\My Documents\OMNIC). This change was necessary to make OMNIC function under Windows Vista but was also a problem for some Windows XP environments.

# History: This file had been used since OMNIC 1.

#### Report notebooks become corrupted when too many reports are added

**Description**: Report notebooks with a very large number of reports were getting corrupted and the reports could not be read/displayed. The number of reports that caused this problem varied depending on how many items were in each report. The incidences of corrupt notebooks that were reported held over 10,000 reports before they were corrupted. The reporting code has been changed to detect when an attempt it made to add a report to a notebook that is near the limit and display an error message. The user must then create a new notebook to save the report.

History: This problem was introduced in OMNIC 3 when report notebooks were introduced.

#### OMNIC no longer allows spectra from commercial libraries to be saved

**Description**: Some previous versions of OMNIC were allowing spectra extracted from commercial libraries to be saved as individual spectral data files (as .spa files, for example). The old restriction that prevents this saving has been reinstated.

#### Series

#### Crash when reopening Rapid Scan series files

**Description**: If a Rapid Scan series file was reopened after the initial collection, the X-axis could be reversed and any manipulation of the data could cause OMNIC to crash. This has been fixed.

# History: This problem was introduced in OMNIC 7.4.

# Sampling Information data and time incorrect for Series data

**Description**: When the option to display the Sampling Information collect time field was turned on, the date and time displayed for Series data was not valid. This has been fixed and is now correct for new series files as well as previously collected series files.

#### History: This problem was introduced in OMNIC 7.3.

#### **Known Issues**

#### OMNIC

#### Tabbing in Options and Experiment Setup does not move between controls.

**Description:** Pressing the tab key does not move the keyboard focus from one control to the next in the Options and Experiment Setup dialog boxes.

**Recommendation:** Use the mouse to move keyboard focus to a control.

History: Problem occurred in all previous versions.

# 960 spectrometer help is not provided.

**Description:** The 960 spectrometer help is no longer included with OMNIC software.

# History: 960 spectrometer help was removed starting with the OMNIC 8.0 release.

#### Uninstalling ValPro causes new SPV features of OMNIC to display errors.

**Description:** If you have OMNIC 8 and ValPro installed and then uninstall ValPro, subsequent use of the System Suitability and Performance Verification features of SPV will display error messages indicating the output files have been tampered with. This is caused by the ValPro uninstaller unregistering the component needed to apply and verify digital signatures.

**Workaround:** Open a command prompt (in Vista be sure to use a command prompt with Administrator rights) and use the command:

regasm "C:\Program Files\Omnic\Thermo\_OMNIC\_XML.dll"

which will re-register the component needed for digital signatures. Note the path to this file may need to be adjusted depending on where the software was installed.

# History: This problem was introduced with OMNIC 8.

#### Macros Pro

# Macro Panel is no longer included with Macros\Pro

**Description**: Macro Panel is no longer included with Macros\Pro<sup>™</sup>. Macros can be added to the OMNIC toolbar with the Edit Toolbar command.

# History: Macro Panel was removed starting with the OMNIC 7.1 release.

#### Series

# TA Instruments TGA file not being read using OMNIC Open TGA Data File command

**Description:** In newer versions of TA Universal Analysis software the file format of the TGA data files was modified so they are not read by OMNIC using the instructions provided. In order for the file to be read by OMNIC it must be saved using the Export utility from the TA software selecting the ANSI character set instead of Unicode.

# History: This bug affects all versions of OMNIC.

# Series 3-D display only shows in black and white

**Description:** With the Radeon x300 or x1300 Pro graphics card, the Series 3D display will not show colors. The workaround to get the image to display in color is to adjust the hardware acceleration setting for the video card. See the Technical Bulletin TBN# IR3140 for detailed instructions on how to do this. This problem can also appear in the Atlµs mapping software.

# History: This bug affects all 7.x versions of Series.

# TA Instruments TGA file not being read using OMNIC Open TGA Data File command

**Description:** In newer versions of TA Universal Analysis software the file format of the TGA data files was modified so they are not read by OMNIC using the instructions provided. In order for the file to be read by OMNIC, it must be saved using the Export utility from the TA software selecting the ANSI character set instead of Unicode.

# History: This bug affects all versions of OMNIC.

# OMNIC DS

# "Run only OMNIC" feature not supported in Windows Vista

**Description**: The security policy named "When user logs on, run only OMNIC" that can be used to prevent selected user groups from having access to the Windows desktop is not supported in Windows Vista.

# History: This is a limitation of Windows Vista support added for OMNIC 8.

#### Screen Saver setting from Thermo Security Administrator not supported in Windows Vista

**Description**: The security policy named "Automatically start screen saver after (minutes)" that can be used standardize a screen saver time for user groups is not supported in Windows Vista.

#### History: This is a limitation of Windows Vista support added for OMNIC 8.

#### OMNIC v7.4.1

#### Resolved Issues

#### International (Non-English) Installation

Some international versions of the Windows operating system have translated Administrator strings that cause a failure when trying to install the OMNIC 7.4 software.

#### OMNIC v7.4

# New Features

# Branding changes

**Description**: Changes have been made to the about box, splash screen, program icons and folder names to reflect the company brand name change to Thermo Scientific. The about box has changed to show the versions from the Windows Installer information rather than the version resources of the actual DLL/EXE files.

# Help Format Change

**Description**: The entire OMNIC help system has been changed to use the "Compiled HTML" help now provided with Windows. There have been some minor changes to the help functionality with this change. For example, right clicking in a spectral window no longer brings up a help window. This change also eliminates problems with .GID files used by the old help system. The old help system tried to update these .GID files as the help file was navigated, but would sometimes display error messages if the user did not have sufficient privileges to update them. If the .GID files did get updated, the modification dates would no longer match what was expected by the IQ tool. These issues are resolved with the new help system.

# Experiment Filename added to list of experiments

**Description**: The dropdown list of experiments has been enhanced to include the filename of the experiment. This helps eliminate confusion when there is more than one experiment with the same title.

# Automatic Atmospheric Suppression improvements

**Description**: Additions were made the Atmospheric Correction feature to improve its performance. This included algorithm changes and an expanded calibration model.

#### Limit on zero fill options with high resolution data

**Description**: A limit on the levels of zero fill the Reprocess feature allowed on high resolution data has been removed. This limit was only needed in 16 bit Windows, but it was left in when the transition to 32 bit Windows was made. Two levels of zero fill are now supported.

# Additional Jasco file types now recognized

Description: Jasco files with a newer binary file type indicator are now read by OMNIC.

# **Resolved Issues**

#### OMNIC

#### Report Notebook spectra all shown in red

**Description**: Reports added to notebooks with versions earlier than OMNIC 7.3 would have spectra all displayed as red when viewed with OMNIC 7.3. This has been changed so only the selected spectrum is displayed in red.

# History: This problem was introduced in OMNIC 7.3

#### **Autosave Base Names**

**Description:** In the Collect tab of Experiment Setup, the drop down list for the Base name in the File Handling box has failed to show the Auto save base names previously used. This has been corrected.

# History: This problem was introduced in OMNIC 7.3

#### Incorrect error message when saving to full disk

**Description:** OMNIC was giving an error message that indicated the target file was write protected if a save was attempted to a disk drive that did not have sufficient free space for the save to succeed. This has been fixed so the error message indicates there is not enough space available.

#### History: This problem occurred in all versions at least back to OMNIC 5.

# Interferograms now attached to reprocessed spectra

**Description:** When some spectra with saved interferograms were reprocessed, the saved interferograms were not attached to the new result spectrum. This has been fixed so copies of the saved interferograms are attached to the newly created result spectrum.

#### History: This problem occurred in all versions of OMNIC.

# Saving data using filenames that include Kanji characters fail

**Description:** OMNIC was not correctly handling filenames that contained some Kanji characters. This has been fixed, but requires a system that is running in Japanese.

# History: This problem occurred in all versions of OMNIC.

#### Derivative command fails from macro if system is language is Japanese

**Description:** The derivative command could fail from a macro if the system was running in Japanese. This has been fixed.

# History: This problem occurred in all versions of OMNIC.

#### QC Compare results not available in Macros Basic

**Description:** The results of a QC Compare operation were not made available in Macros Basic. This has been fixed.

# History: This problem occurred in all versions of OMNIC since OMNIC 3.

# Library Converter now allows output to be put in same directory as input

**Description:** The Library converter program would generate errors if the output library was written to the same directory as the input file. This restriction has been removed.

# History: This problem occurred in the LibConverter provided with OMNIC 7.3

#### Data from some GRAMS format libraries scaled incorrectly by Library Converter

**Description:** The data from some GRAMS format libraries was being scaled from 0 to 256 instead of from 0 to 1.0. This has been fixed

# History: This problem occurred in the LibConverter provided with OMNIC 7.3

#### Data that cross zero on X Axis may crash Find Peaks

**Description:** Spectra with data that spanned zero on the X Axis could cause Find Peaks to crash. This has been fixed

#### History: This problem occurred in all versions of OMNIC since OMNIC 3.

#### Paste operation fails on newly created window

**Description:** When a paste was done into a newly created window, the focus was on the disabled title control rather than on the spectral display, so the paste operation failed. This was fixed by programmatically setting the focus on the spectral window.

#### History: This problem occurred in all versions of OMNIC since OMNIC 7.

#### Autosave sequence number does not always increment from a macro

**Description:** Collects done in a macro would sometimes overwrite previous collects because the autosave sequence number was not incremented. This only failed from macro collects and has now been fixed.

# History: This problem was introduced in OMNIC 7.2

# Message displayed indicating intermediate collect results would not be displayed

**Description:** Collects of high resolution data (0.125 cm-1) would display a message indicating the result would not be displayed until the entire collect was complete, but the intermediate results would in fact get displayed. This message has been removed.

# History: This problem was introduced in OMNIC 5

#### Bench and Diagnostic Tabs of Experiment Setup don't center peak

**Description:** When changes were made in Experiment Setup that caused the collect used to populate the interferogram display to change sample spacing, the region of the interferogram displayed was not adjusted to focus on the same features. This would usually cause the peak to be outside of the display region. This has been changed so the displayed region is adjusted for sample spacing changes.

# History: This problem was introduced in OMNIC 4

# File Open dialog locks up opening some Mattson files

**Description:** OMNIC would lockup when trying to read some files in the Mattson WinFirst format. This happened on files that had text annotations. This has been fixed so the files read correctly.

# History: This problem was introduced in OMNIC 6

# Pasting Search results into Log file gives garbled RTF

**Description:** If a copy was done from an OMNIC window that produced tabular results and then the table was pasted into OMNIC's log file, the table header would be garbled. This was fixed by using spaces instead of tabs in the all of OMNIC's table headers.

#### History: This problem was introduced in OMNIC 7.2

#### Floating-Point overflow when expanding interferogram display in Experiment Setup

**Description:** A floating-point overflow would sometimes occur when expanding the interferogram display on the Bench tab of Experiment Setup, causing an error message to appear that forced the user to close OMNIC. This has been fixed.

#### History: This problem was introduced in OMNIC 7

#### Raman menu shown twice

**Description:** If OMNIC had trouble communicating with the instrument at startup, but then was able to establish good communications, the Raman menu would end of being added to the top level menu twice. Some of the items in the two menus would then be enabled/disabled at the wrong times. This has been fixed.

#### History: This problem was introduced in OMNIC 6.2

#### Collect Sample with region selected stops update

**Description:** In the data collect window, if the region tool was used to define a region, the remainder of the collect would be discarded and the spectrum on display at the time the region was defined would be used as the final result. This was true even if the region was defined while the background single beam was being collected. This has been fixed.

# History: This problem was introduced in OMNIC 7.3

#### **Known Issues**

# OMNIC

#### Uninstalling OMNIC 7.x on a system that was upgraded from OMNIC 6.1a

**Description**: If you install OMNIC 7.x over a OMNIC 6.1a installation and then try to uninstall OMNIC 7.x using either the Uninstaller on the OMNIC 7.x CD or from Add/Remove programs, the OMNIC exe's and dlls are not removed. The reason is that OMNIC 6.1a was not uninstalled before OMNIC 7.x was installed. To uninstall v6.1a, run the uninstaller in the /uninstall folder.

# History: This behavior was introduced with OMNIC 7.0.

# Tabbing in Options and Experiment Setup does not move between controls.

**Description:** Pressing the tab key does not move the keyboard focus from one control to the next in the Options and Experiment Setup dialogs.

**Recommendation:** Use the mouse to move keyboard focus to a control.

**History:** Problem occurred in all previous versions.

#### Macros Pro

# Macro Panel is no longer included with Macros\Pro

**Description**: Macro Panel is no longer included with Macros\Pro<sup>™</sup>. Macros can be added to the OMNIC toolbar with the Edit Toolbar command.

# History: Macro Panel was removed starting with the OMNIC 7.1 release.

#### Series

# TA Instruments TGA file not being read using OMNIC Open TGA Data File command

**Description:** In newer versions of TA Universal Analysis software the file format of the TGA data files was modified so they are not read by OMNIC using the instructions provided. In order for the file to be read by OMNIC it must be saved using the Export utility from the TA software selecting the ANSI character set instead of Unicode.

# History: This bug affects all versions of OMNIC

# Series 3D display only shows in black and white

**Description:** With the Radeon x300 or x1300 Pro graphics card, the Series 3D display will not show colors The workaround to get the image to display in color is to adjust the hardware acceleration setting for the video card. See the Technical Bulletin TBN# IR3140 for detailed instructions on how to do this. This problem can also appear in the Atlµs mapping software.

# History: This bug affects all 7.x versions of Series.

# OMNIC v7.3 Service Pack 1 (SP1)

# **New Features**

# Change to version numbers shown in About box

**Description**: A change to the approach used to deliver maintenance software releases for OMNIC related products resulted in a change to the information shown in the About OMNIC box in the Help menu. Maintenance releases for OMNIC related products are being issued as Service Packs that bundle files for all products that have been changed. Only the specific files that have changed are updated by the new service pack installation process. There will no longer be maintenance releases of individual components, such as OMNIC Search. Because of this, the third component of the version number (such as the 'a' in 7.2a) is no longer used. Instead, the latest service pack (which applies to all components) is shown near the top of the About box.

It should be noted that the Service Pack installation requires OMNIC 7.3 to be installed on the computer.

# Support of the Nicolet 8700 (USB version)

**Description**: Support has been added for the USB version of the Nicolet<sup>™</sup> 8700 spectrometer. This includes the extension of the PM modulation amplitude to 4.5 lambdas and three enhancements of step-scan time-resolved data collection: The optional use of an additional input (Sync), a shorter (1 microsecond) minimum sampling interval when using the spectrometer digitizer, and the ability to use multiple triggers per step when using the spectrometer digitizer.

# New correlation options avoid shifting first scan of collect

**Description**: Two new correlation options were added that are available only by setting the DDE parameter "Collect Correlation" to "NoPeakShift" or "NoShiftSimple". These settings cause OMNIC to assume the instrument positioned the peak at the exact location requested for

the first scan and do not shift the scan. All previously existing correlation options shift the first scan so the largest peak (in absolute value) is located at the requested position. The "NoPeakShift" option does not do any correlation on subsequent scans, while the "NoShiftSimple" option still does simple correlation on subsequent scans.

This was done to provide a work around for unusual collect conditions where the ZPD location cannot be inferred from the largest peak.

#### **Resolved Issues**

### OMNIC

#### Smart Accessories not recognized in some circumstances on Nicolet 380 and x700

**Description**: OMNIC was not responding to insertion and removal of Smart Accessories<sup>™</sup> if the instrument had not been used to collect data for more than 40 minutes. A change was made so the instrument always responds to smart accessory changes if OMNIC is running. If OMNIC is not running, the instrument will still go into a "rest mode," but starting OMNIC will automatically take the instrument out of "rest mode."

#### History: This problem was introduced in OMNIC 7.3

## Nicolet 6700 with Dual Channel option does not collect correctly

**Description**: OMNIC 7.3 has reversed the A and B channels on Nicolet 6700 Dual Channel systems. Channel B on these systems is suppose to be the BNC mounted in the baseplate to the right of the sample compartment. When OMNIC 7.3 is loaded, this becomes Channel A. Then when a Dual Channel PEM collect is made the spectral data that is automatically ratioed will be upside down. This has been fixed.

# History: This problem was introduced in OMNIC 7.3

# Spectral Header information not correctly extracted from user libraries

**Description**: If a spectrum is added to a user library created with OMNIC 6.0 or newer, the header information is preserved in the library and can be viewed if the spectrum is extracted from the library. However, a bug in extracting the spectrum from the library was causing this header information to be lost. Because of this, using a spectrum extracted from a user library as input to the "Match Spectrum Settings" command on the Collect menu would not result in the settings being set to match those used to collect the library spectrum. This has been fixed so that the correct header information is extracted from user libraries.

#### History: This problem was introduced in OMNIC 7.2

#### Check Desiccant button not available for Nicolet 380 systems

**Description:** The Check Desiccant button on that is suppose to appear on the Diagnostic tab of Experiment setup was not present on Nicolet 380 systems. This has been changed so the button appears and functions.

# History: This bug was introduced in OMNIC 7.1 when support was added for the Nicolet 380.

#### Align results in flat line interferogram on 460 and ECO 1000

**Description:** On some 460 and ECO<sup>™</sup> 1000 systems, using the Align feature on the Diagnostic tab of Experiment Setup would appear to work correctly, but at the very end of the Align, the interferogram would change to a flat line. A Reset of the bench would restore correct

scanning operation. A driver change was made to add a small delay (10 milliseconds) to the end of the Align operation to avoid this problem.

# History: This bug was introduced in OMNIC 7.0

#### Polarizer wheel does not move to zero on a Nicolet 8700

**Description:** A bug was found in the Nicolet 8700 PCI driver which prevented the polarizer wheel from moving to zero if the attenuation wheel was at zero. This has been fixed

#### History: This bug was introduced in OMNIC 7.3

#### Company Logo change on EZ OMNIC Splash Screen

**Description:** The company logo on the EZ OMNIC splash screen was changed from the Thermo Nicolet logo to the Thermo Electron logo. This change was missed when the OMNIC splash screen changes for version 7.0.

#### History: This bug was introduced in OMNIC 7.0

#### Find Peaks locks up if spectrum X Axis crosses zero

**Description:** The Find Peaks operation on the Analyze menu may cause OMNIC to lock up if the X Axis covers a range of both positive and negative values. This has been fixed. A work around that avoids this lock up is to manually add a piece of annotation using the text tool prior to doing the Find Peaks.

# History: This bug was introduced in OMNIC 7.3

#### **Macros Basic**

#### Macros Basic problems with comma for decimal point

**Description:** Macros Basic was not handling floating point numbers correctly if the system was set to use the comma as a decimal point character. This bug has been fixed.

History: This bug has existed since at least OMNIC 6.2.

#### Some Macros saved in Chinese cannot be reopened

**Description:** Some Macros Basic macros saved on systems using Chinese as the system language could not be reopened. This has been fixed.

# History: This bug was introduced in OMNIC 7.3

#### Series

#### Incorrect date/time shown for Rapid Scan data.

**Description:** Data collected with Rapid Scan show incorrect date/time in the Series Information window. This is for the "collected" date in the second line and also for the "data processing" section in the history. The year shows up as 2036 and the month/date appear are arbitrary. This has been fixed.

#### History: This bug was introduced in OMNIC 7.3

#### Rapid Scan for 380 uses wrong Settle time

**Description:** The settle time used for Rapid Scan runs on a 380 was too short causing poor quality data to be collected. The settle time was changed from 2 milliseconds to 200 milliseconds for the 380.

# History: This bug was introduced in OMNIC 7.3

# Using more than three Quant components in a Series run causes problems

**Description:** If more than three quant components were selected for profiles using a selected quant method when collecting Series data, the Y Axis labels of the profiles could be displayed incorrectly and crashes could occur. This has been fixed.

# History: This bug was introduced in OMNIC 7.3

# Series window can now be closed from DDE without prompt to save data

**Description:** The CloseWindow DDE command can be issued with the argument "Yes" to save changes to data automatically without prompting the user (that is, "CloseWindow Yes"). The Series window now recognizes this argument and will close without a prompt if it is present. This allows a Series run to be stopped before is completes by using the two commands "StopCollect" and "CloseWindow Yes".

# History: This bug was introduced in OMNIC 7.3 because Series data is no longer written to disk as operations are performed.

# GC temperatures not sent to instrument when changed in Experiment Setup

**Description:** Changes made to the GC flow cell and transfer line temperatures were not being sent to the instrument when they were changed in Experiment Setup. This has been fixed.

# History: This bug was introduced in OMNIC 7.3

#### Rapid Scan on 8700 PCI misses scans

**Description:** Rapid Scan data collected on an 8700 PCI would have gaps where scans were missed if Smart Accessory polling was not manually turned off during the run. This was fixed by automatically turning off polling of Smart Accessories during a Rapid Scan run for 8700 PCI instruments and restoring the previous polling state at the end of the run.

# History: This bug was introduced in OMNIC 7.3

# Timing of Series collect with external trigger starts before trigger

**Description:** The duration of a Series collect started with an external trigger could be shorter than expected because the collect timer was being started before the trigger occurred. This has been fixed so the collect time does not start until the trigger occurs.

# History: This bug was introduced in OMNIC 7.3

# Generation of CNC file for profiles created post analysis

**Description:** The concentration output text file (CNC) would not get generated when creating a profile on an existing Series data file. This has been fixed so the file now gets generated in this mode.

# History: This bug was introduced in OMNIC 7.3

#### **Known Issues**

# OMNIC

# Uninstalling OMNIC 7.x on a system that was upgraded from OMNIC 6.1a

**Description**: If you install OMNIC 7.x over a OMNIC 6.1a installation and then try to uninstall OMNIC 7.x using either the Uninstaller on the OMNIC 7.x CD or from Add/Remove programs, the OMNIC exe's and dlls are not removed. The reason is that OMNIC 6.1a was not uninstalled before OMNIC 7.x was installed. To uninstall v6.1a, run the uninstaller in the /uninstall folder.

# History: This behavior was introduced with OMNIC 7.0.

#### Tabbing in Options and Experiment Setup does not move between controls.

**Description:** Pressing the tab key does not move the keyboard focus from one control to the next in the Options and Experiment Setup dialogs.

**Recommendation:** Use the mouse to move keyboard focus to a control.

**History:** Problem occurred in all previous versions.

#### Macros Pro

#### Macro Panel is no longer included with Macros\Pro

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# History: Macro Panel was removed starting with the OMNIC 7.1 release.

# Series

# TA Instruments TGA file not being read using OMNIC Open TGA Data File command

**Description:** In newer versions of TA Universal Analysis software the file format of the TGA data files was modified so they are not read by OMNIC using the instructions provided. In order for the file to be read by OMNIC it must be saved using the Export utility from the TA software selecting the ANSI character set instead of Unicode.

#### History: This bug was affects all versions of OMNIC

#### OMNIC DS Data Security

# Require Signature When Saving Spectrum and OMNIC for Almega

**Description:** If **OMNIC DS Data** Security is **installed** on your system, the **Require Signature When Saving Spectrum** policy should be disabled during instrument calibration and when smart background data are due to be collected so that the collections will not be interrupted by requests for **digital** signatures. Smart background data are collected during the first ~40 hours of instrument inactivity after **OMNIC for Almega**<sup>™</sup> 7.3 is installed and periodically after that based on the setting of the Maximum smart background age control in the Calibrate Instrument dialog.

# OMNIC v7.3

### **New Features**

# OMNIC

# Added capability to read Bruker and Jasco spectral files

**Description**: OMNIC can now open and display Bruker [.0-9]\* and Jasco [\*.JWS] spectral data files.

# History: This is an enhancement for 7.3

# Conversion of PerkinElmer, Bruker, GRAMS/Spectral ID & Sadtler SearchMaster libraries

**Description**: A new application titled "Library Converter" has been developed to convert PerkinElmer<sup>®</sup> Spectrum, Bruker OPUS<sup>®</sup>, GRAMS/Spectral ID<sup>TM</sup> and Sadtler<sup>TM</sup>

SearchMaster<sup>TM</sup> user libraries to OMNIC format. The converted libraries can then be used in OMNIC for library searching and with the Library Manager feature.

# History: This is an enhancement for 7.3

#### New interactive Kramers-Kronig correction

**Description**: A new processing function has been added which allows the user to convert specular reflectance data with a Kramers-Kronig correction and either normalize the result to 1 (one) Absorbance unit or 1 (one) micrometer. The user can also choose to have the N-index and/or the K-index spectrum appear with the result.

# History: This is an enhancement for 7.3

# Ability to set the parameters for automatic baseline

**Description**: The polynomial order and number of iterations for the automatic baseline function can be set in the Edit/Options/Process Tab.

# History: This is an enhancement for 7.3

# Added the ability to apply a linearization method to photoacoustic data

**Description**: A new processing function titled "PAS Linearize" has been added that will apply the linearization method of R.O. Carter III, Applied Spectroscopy, 46, 219, 1992) to the data. This enhances the infrared signal at the sample surface and improves quantitative linearity.

History: This is an enhancement for 7.3

#### Titles of the spectra in the search list are now displayed in overlay mode

**Description**: In previous versions, titles for the spectra in the search list were only displayed if the spectra were stacked. Titles are now also displayed if the spectra are in overlay mode.

# History: This is an enhancement for 7.3

# Added the ability to include the name of a notebook in a report

**Description**: Previously, a field did not exist to add the name of a notebook to a report. This field has now been added.

# History: This is an enhancement in 7.3

#### Clipboard button added to Search Results window

**Description**: A clipboard button was added to the Search Results window that copies the hit list as a text table as well as the graphical display of the search results. Users can use "Paste Special" in most programs, such as MS Word, to select the format of data they want to paste.

#### History: This is an enhancement in 7.3

# Tabular data written to Clipboard as RTF

**Description**: Many places in OMNIC that write tabular data to the clipboard were changed to write the data as an RTF table as well as the previously supported unformatted text. Users can use "Paste Special" in most programs, such as MS Word, to select the format of data they want to paste. Pasting RTF tables can simplify formatting of the information in external documents. RTF tables are now produced for Find Peaks, Peak Resolve, Search Results, and Annotations,

# History: This is an enhancement in 7.3

# **OMNIC** can control Antaris model spectrometers

Description: OMNIC can now be used to control the Antaris and Antaris IGS spectrometers.

# History: This is an enhancement for 7.3

#### Series

# Series data collect has been updated

**Description**: Setting up a series data collection is no longer done through the Series menu; it has been fully integrated into OMNIC's Experiment Setup dialog. If Series is installed on your system, a new tab titles "Series" will appear in the Experiment Setup dialog. The previous capabilities of configuring a series data collection are still available. Additionally, new functionality has been added to setting up a series data collection including the ability to set collect data for a specific period of time, delay (or suspend) collect data during a specific time period, collect data until a specified intensity value is attained, or delay (or suspend) data collection until a specific intensity value is reached. The user can also set the Y-axis range for the series data collection.

# History: This is an enhancement for 7.3

# Series supports FT-Raman and dispersive Raman spectrometers

**Description**: Series data collection can now be used with FT-Raman and Almega<sup>TM</sup> spectrometers.

# History: This is an enhancement for 7.3

# Opening and saving series data files has been updated

**Description**: Opening and saving series files is now done through the OMNIC File menu Open, Save, and Save As items.

# History: This is an enhancement for 7.3

# Series 3D display features has been enhanced and updated

**Description**: Displaying a series file with the "Show Series 3D window" menu item has been completely redone. A new interactive 3D display is available that allows the user to change the viewing angle of the image with the mouse. An enhanced 2-D contour plot has been added. A color bar has been added to allow the user to change the color palette used in the 2D and 3D images to better differentiate differences in the series data file. Additionally, the user can view the spectra and/or profiles on the same screen. The four panes are interconnected so that selecting a point or spectrum on one pane, updates the other panes correspondingly. Right-click pop-up menus are connected to each pane for quick access to common features of that pane.

# History: This is an enhancement for 7.3

# Enhanced display options for series data profiles

**Description**: Users have the option to set up to 10 profiles with each series data collect. Previously, the limit was 3 (three). Profiles can be displayed in either overlay or stack mode. Through the right-mouse pop-up menu, users can choose to copy individual or all profiles to an OMNIC spectral window. A similar copy and paste functionality has been added for spectra.

# History: This is an enhancement for 7.3

# Processing of Series files is integrated into OMNIC menus

**Description**: Users can now use the Process menu to apply relevant processing functions (absorbance, transmittance, other conversions, reprocessing (with saved interferograms), automatic baseline correct, other corrections, blank, straight line, subtract, automatic region subtract, smoothing, derivative and multiply). In previous releases, these functions where applied through the Apply Function menu item in the Series menu.

# History: This is an enhancement for 7.3

#### Searching of a spectrum from a series data collect

**Description**: Users can search the selected the spectrum in the series window. There is no longer a need to first copy the spectrum to an OMNIC spectral window.

# History: This is an enhancement for 7.3

#### Saving of intermediate data during a series collect

**Description**: During a series data collect, data is always saved to disk after every collect cycle in order to prevent data loss in case of an error or power failure.

# History: This is an enhancement for 7.3

# Ability to use basis vectors from a saved file

**Description**: Users have the option to use basis vectors from a specified file versus collecting them at the start of a series collection. Also, the basis vectors can be used as the background rather than collecting a separate background. This can speed up the time of the series data collection.

# History: This is an enhancement for 7.3

# Interferograms can be saved during a series collection

**Description**: Users have the option to save the interferograms along with the data in a series collection. Interferograms must be saved if the user desires to reprocess the series data set.

# History: This is an enhancement for 7.3

#### Split series supports long file names

**Description**: Users use up to 64 characters for the names of the individual files created when splitting a series file. In previous versions, the limit was 4 characters.

# History: This is an enhancement for 7.3

# Series features supported by Thermo Security Administration

**Description**: Access to the Series features and policies for series spectral data files can now be controlled with the Thermo Security Administration application if needed by the user to comply with FDA regulations such as 21 CFR Part 11.

# History: This is an enhancement for 7.3

# EZ OMNIC

# Automatic Atmospheric Suppression now supported in EZ OMNIC

**Description**: Atmospheric suppression can now be used in EZ OMNIC to automatically remove water vapor and CO2 interferences during spectral data collection.

# History: This is an enhancement for 7.3

#### Advanced ATR now available

Description: Users can now apply the Advanced ATR Correction processing feature.

#### History: This is an enhancement for 7.3

#### EZ OMNIC now supported by DS and Thermo Security Administration

**Description**: The ability to digitally sign spectral data files in EZ OMNIC and control EZ OMNIC through Thermo Security Administration has been added. Note it cannot be used to sign library files in EZ OMNIC.

#### History: This is an enhancement for 7.3

#### Print/Preview Report is available

**Description**: Users now have the ability to print and preview reports with EZ OMNIC. A variety of templates are provided for including the spectral data, search results, peak tables, and data collection information together in a single document which can then be printed.

#### History: This is an enhancement for 7.3

# Software IQ

#### New application provided with OMNIC DS to verify software installation

**Description**: A new application is available with OMNIC DS to verify that the correct versions of files are installed and that the files are installed in the correct folders. A report in HTML format is generated that lists all of the installed files and notes any discrepancies from the expected result. This replaces the written checklist of files previously provided for OMNIC and OMNIC DS Software IQ.

#### History: This is an enhancement for 7.3

#### **Resolved Issues**

#### OMNIC

# Selected spectra not retained when added to a notebook

**Description**: If multiple spectra existed in a spectral window when the data was added to a notebook, which spectrum was the selected spectrum was not retained in the notebook itself. This has been changed so that the selected spectrum from the spectral window appears as the selected spectrum when the report is viewed in the notebook.

#### History: This has existed since lab notebook functionality was added with OMNIC 4.0

#### Title of a newly created notebook was incorrect when the notebook was viewed

**Description**: Create a new notebook. Use the View Notebook command and choose a different notebook to view. From viewing notebook window, choose the newly created notebook. The title displayed when the new notebook appeared was that of the previously viewed notebook. This has been changed to show the title of the currently selected notebook.

# History: This has existed since lab notebook functionality was added with OMNIC 4.0

# Displayed data collection information is not added to the report in a notebook

**Description**: If the data collection date and time were displayed in the OMNIC spectral window and the data was added to a notebook, the collection date and time did not appear in the spectral window in the notebook report. This had been changed so that the displayed collection information is displayed in the report notebook if it appears in the spectral window.

# History: This has existed since lab notebook functionality was added with OMNIC 4.0

#### The base file name for autosave has been expanded to 32 characters

**Description**: In previous versions of OMNIC, the length of the base file name for autosave was limited to 4 characters. This has been increased to support up to 32 characters.

# History: This has existed in all previous versions of OMNIC

#### The down arrow control for viewing the list of spectra disappeared after hiding a spectrum

**Description**: On some systems, the down arrow next to the list for the spectra in the OMNIC window disappeared after hiding a spectrum. This prevented the user from "unhiding" the hidden spectra. This has been fixed.

#### History: This has existed on some systems since OMNIC 6.1a

#### Cannot not label peaks or pick peaks if spectra are in wavelength

**Description**: Peaks could not be annotated correctly if the x-axis was in wavelength. This has been fixed to show the correct annotation for the selected x-axis.

#### History: This has existed in all previous versions of OMNIC

#### Could not print out entire list of QC Compare libraries if greater than one page

**Description**: Printing out a listing of all QC Compare libraries would stop after the first page. This has been fixed to print out all QC Compare libraries using multiple pages if needed.

# History: This has existed since OMNIC 4.0

#### Auto file naming spectra in a macro could give odd file names

**Description**: If the base file name for autosaving spectra in a macro ended in a number, the names would not sequence correctly. This has been fixed to allow base file names to end in alphabetical or numeric characters.

#### History: This has existed in all previous versions of OMNIC

#### Selecting a new initial library directory in Options was not seen in Library Setup

**Description**: If a different Initial User Library directory was set in the Edit/Options/File dialog, the directory didn't appear in the Library Directories box in Library Setup. To see it, one had to delete one or more of the listed directories from the box. This has been fixed to include the initial user library directory in the list of Library Directories in Library Setup.

#### History: This has existed since OMNIC 6.1

#### Y-axis annotations are fixed at 3 decimal points

**Description**: The number of decimal points use for Y-axis annotations is now controlled by the number of decimal points option in the Options dialog.

# History: This has existed in all previous versions of OMNIC

# If region search is used, the regions are not displayed in the Search Result window

**Description**: Search regions were not displayed on the Search Result window if they were enabled. OMNIC has been changed to display the search regions on the results window.

#### History: This has existed since OMNIC 7.0

# Copying and pasting an OMNIC window with a selected area does not display the region correctly in MS Word

**Description**: If a spectral window showing a shaded area is copied and pasted into Microsoft<sup>®</sup> Word, the shaded area extends past the bottom of the y-axis. This has been changed to only show the shaded area with the boundaries of the graph.

#### History: This has existed since OMNIC 7.0

# The options in the bench tab of experiment setup are not properly updated if a Smart Accessory is changed

**Description**: If a Smart Accessory<sup>TM</sup> change is made when the Bench Tab of Experiment Setup is open, the dialog settings are not updated. The Smart Accessory change will cause a new experiment file to be loaded, but the new settings are not shown in the Bench tab. Also, the live display does not properly show the interferogram. This has been changed to properly update the Bench tab settings with the information from the newly loaded experiment file.

# History: This has existed since OMNIC 7.0

# If match settings is used in Library Manager to collect a spectrum, it does not follow the options set for number of background scans

**Description**: Spectra collected by selecting match settings in Library Manager always collected the same number of background scans as sample scans. It ignored whether a different number of background scans had been enabled in the Collect tab of Experiment. This has been changed to follow the settings in the Collect tab.

# History: This has existed since OMNIC 7.0

# Autoblanking regions can cause Advanced Diagnostics tests to fail

**Description**: If autoblanking regions were enabled in the Advanced Tab of Experiment Setup, the regions were used during the advanced diagnostics tests. If the region between 2000 and 100 was blanked, the tests would fail. This has been changed so that advanced diagnostics ignores the autoblank regions.

#### History: This has existed since OMNIC 7.2

#### Spectral range for the diamond Smart Orbit gives improper out-of-range warnings

**Description**: The diamond window material range and useful range for the Smart Orbit differ and a warning is displayed if the range is set to go below the recommended range of 525 cm-1 for diamond. This has been changed to allow for the full range of the diamond optics.

#### History: This has existed since OMNIC 7.2

#### Default report template not set at install

**Description**: A default report template was not set up when the software was installed. This has been changed to load a default template.

# History: This has existed since OMNIC 7.2

# When the information produced with the region tool is removed after the region is drawn

**Description**: While the region tool is used to draw an area, it displays information about the selected region. The information disappears as soon as the drawing is complete although the shaded region remains. This has been changed to show the information with the shaded region.

# History: This has existed in all previous versions of OMNIC

# Messages of inappropriate parameters in the experiment file do not indicate which parameter was incorrect

**Description**: If an experiment file is opened and a parameter from the experiment is not appropriate for the current system configuration, a generic error message would appear saying an inappropriate parameter was found and not loaded. This has been changed to identify which parameter was not appropriate.

# History: This has existed in all previous versions of OMNIC

# OMNIC may crash when reprocessing libraries created with OMNIC 6

**Description**: If a version 6 OMNIC library was reprocessed through DDE, OMNIC may crash. This was fixed to allow the reprocessing on OMNIC 6 spectra.

# History: This has existed since OMNIC 7.2

# EZ OMNIC

# Selecting an \*.spa file in Windows Explorer and double-clicking does not launch EZ OMNIC

**Description**: On systems with only EZ OMNIC installed, the application would not launch if a spectral data file was double-clicked in Windows Explorer. This has been fixed.

# History: This has existed since OMNIC 6.1

# A default experiment file is not selected during the installation

**Description**: A default experiment file is not set when EZ OMNIC is installed. This has been changed to load default.exp when EZ OMNIC is first installed.

# History: This has existed since OMNIC 7.2

# Val-Q<sup>™</sup> autotester will not run with EZ OMNIC

**Description**: The auto tester program for algorithm verification would not run on EZ OMNIC only systems. This has been fixed.

# History: This has existed since OMNIC 7.1

# Peak Resolve

# Wrong peak may be highlighted when editing peak table

**Description**: After a fit operation, the peak table can be viewed in the Peaks... dialog. It was possible for the wrong peak to be highlighted in the graphical window behind the dialog. This has been changed so the correct peak is highlighted.

# History: This has existed since OMNIC 7.2

# Thermo Security Administration

# Access to adding a library spectrum to a window is not totally controlled with Thermo Security Administration

**Description**: If Thermo Security Administration was used to disable access to the library manager "Add to window" button, it only turns it off on the Library tab. The same button on the Spectra tab is still enabled. This has been changed so that if access to the Add to Window functionality is disabled, it is disabled on both tabs of Library Manager.

# History: This has existed since OMNIC 6.2

# Report templates could be overwritten when prevent overwriting files was enabled in Thermo Security Administration

**Description**: Even with the policy set to prevent overwriting on files, report templates could be overwritten as Save As was enabled with the Edit template feature. This has been changed to disable the Save As functionality if prevent overwrite files is enabled.

# History: This has existed since OMNIC 7.1

# Thermo Security Administration allows any valid user to log in

**Description**: When the Thermo Security Administration program starts, it prompts for a user name and password. However, it accepts any valid username and password rather than just the person for the currently logged on user. This has been changed so that only the person currently logged on to the computer can log into Thermo Security Administration.

# History: This has existed since OMNIC 7.2

# Thermo Security Administration fails to add domain user to policy groups

**Description**: Under some conditions, after a local user account has been added to a policy group, all attempts to add domain user accounts will fail. This has been fixed.

# History: This has existed since OMNIC 6.2

# Unable to sign files a second time if prevent overwriting is enabled

**Description**: If the Thermo Security Administration program has prevent overwriting of files enabled, the user who collected the spectrum or another user will not be able to sign the file again. The user will receive the error: "Write denied. The file is read only." This has been changed to allow the user to sign the files more than once.

# History: This has existed since OMNIC 7.2

# Additional Analyze menus items are being disabled

**Description**: If access is denied to everyone for the last entries of the Analyze menu (Quantify, Quant Setup, and View Library), "Add to Library" command is also disabled. In addition if the permission to access "Add to Library" is removed the "QC compare" function is disabled as well. This has been changed to only disable the selected features.

# History: This has existed since OMNIC 7.2

OMNIC v7.2a

# **Resolved Issues**

# OMNIC

# Font used for axis on printed reports very small or very large

**Description**: An intermittent problem with the size of the font used for printing axis in reports was fixed. Reports now print with the correct axis font.

# History: This has been a bug since reports were added to OMNIC in version 3.0.

# Bitmaps that overlap other fields of report fail to print

**Description**: On some printers, bitmap fields of reports will not print out if they overlap other fields. A warning message is now displayed when a report template is saved and there is an overlapped bitmap field that may not print on some printers. Users can choose to save the template anyway since the report will print correctly on most printers.

# History: This issue is related to printer drivers and could occur in any version of OMNIC that includes reporting (version 3.0 and later).

# Printing to non-Default printer may use incorrect font size

**Description**: Any printout in OMNIC that was sent to a printer other than the default printer would use the wrong size fonts if the selected printer was set for a different DPI than the default printer. This is similar to the report printing bug mentioned above, but could affect any printed text in OMNIC and was not intermittent on systems configured as described. The problem has been fixed by selecting the correct fonts for the printer selected.

# History: This has been a bug in all previous versions of OMNIC.

# Username provided to ValPro not correct

**Description**: If OMNIC was not configured for logins (either with OMNIC DS or OMNIC custom logins), the username OMNIC provides to ValPro<sup>™</sup> was the name entered when OMNIC was installed rather than the name of the current user. This results in the ValPro report displaying the incorrect username. This has been fixed so that OMNIC now provides the name of the user currently logged on to Windows.

# History: This problem was introduced with OMNIC 7.2 and the initial release of the ValPro product.

# Access Violation when collecting data from a Macros\Basic macro

**Description**: An occasional Access Violation would occur when repeatedly running a Macros\Basic<sup>™</sup> macro that collected data and the macro was set to "Reset OMNIC parameters when macro ends". This same problem would sometimes cause the spectra to draw with a "filled" appearance. The problem has been fixed in this release.

# History: This problem was introduced with OMNIC 7.0

# Y Axis label incorrect when importing some Perkin-Elmer files

**Description**: Perkin-Elmer files that used a Y-Axis identifier of "Abs" rather than "A" were displayed in OMNIC with a Y-Axis label of "Arbitrary Units". OMNIC now recognizes these files as absorbance and displays the correct Y-Axis label.

# History: This problem has existed in all versions of OMNIC that read Perkin-Elmer files.

# Access Violation when setting up Atmospheric Correction

**Description**: An access violation would occur when using Experiment Setup to create an experiment file that used Atmospheric Correction and a set of collect options not covered by the supplied correction standards. The violation occurred when OMNIC tried to generate the new standards needed for unusual collect conditions, such as triangular apodization. Most of these unusual collect conditions are controlled on the advanced tab of Experiment Setup. This problem has been fixed.

# History: This problem was introduced with OMNIC 7.0.

# Atmospheric Correction controls disabled in EzOMNIC

**Description**: Atmospheric Correction is not included in EzOMNIC, but some of the controls in Options and Experiment Setup that are used to control this feature are still enabled. This has been changed so the controls are disabled in EzOMNIC.

#### History: This problem was introduced with OMNIC 6.1.

#### OMNIC DS

#### Save Group (.SPG) does not generate an event log record

**Description**: The Save Group operation in OMNIC that writes .SPG files was not generating an event in the Thermo portion of the Windows Event Log. This has been fixed.

#### History: This problem was introduced with OMNIC 6.2.

OMNIC v7.2

#### New Features

# OMNIC

#### ValPro compatibility

**Description**: Features have been added to OMNIC to support the new ValPro validation package.

#### History: This is an enhancement for 7.2

# OMNIC DS

#### Individual control of ancillary OMNIC programs launched from OMNIC

**Description**: Access to all of the ancillary programs that can be launched from the OMNIC menus can now be controlled individually from the Thermo Security Administration (TSA) program. This allows administrators to restrict a given user to launching some ancillary programs but not others. For example, a user may be allowed to launch Advanced Diagnostics, but not allowed to launch ValPro. In previous versions, the ability to launch all ancillary programs, as well as independent programs assigned to toolbars or menu items through Edit Toolbar or Edit Menu were controlled by a single access control item in TSA (called "Run programs from menu or toolbar" in the "Custom toolbar and menu items" group).

To gain access to these new settings in TSA, the administrator must load the new OMNIC.XML file through the "Add Application..." menu item in the File menu of TSA. The OMNIC.XML file is located on the root of the OMNIC installation CD in uncompressed format. Loading the new version will only add new entries to the TSA database; it will not change any existing settings.

The new entries are located in the Access Control group that corresponds to the OMNIC menu they appear in. For example, Advanced Diagnostics is in the Collect group and InterpretIR+<sup>™</sup> is in the Analyze group.

The "Run programs from menu or toolbar" access control item mentioned above is still available for controlling access to all independent programs added to the menu or toolbar.

If you are upgrading to version 7.2 of OMNIC DS and do not reload the OMNIC.XML file into TSA, all of the ancillary programs will be controlled by the "Deny access to menu items not in security database" System Policy since OMNIC now sees each of these as an individual command rather than a run command.

# History: This is an enhancement for 7.2

# **MACROS PRO**

#### Environment variables can be used in arguments

**Description**: OMNIC now expands all environment variables in DDE arguments before executing the commands. This also occurs when the commands are passed through the OMNIC COM interface.

#### History: This is an enhancement for 7.2

#### New "Locked" mode available for the OmnicMode command

**Description**: The OMNIC Macros Pro DDE command "OmnicMode" now accepts the "Locked" keyword to put OMNIC in a mode similar to the "Simple" mode with no menus or toolbars, but with the additional constraint that user input is ignored on the active window. This prevents the user from changing the active window or boxing within the active window or any other similar interactions. However, dialogs that are presented by OMNIC do accept user input. This new mode can be used when OMNIC is being driven by an external program or macro to prevent users from making unwanted changes to the context OMNIC is using. To switch back to the normal mode, use the command "OmnicMode Normal".

# History: This is an enhancement for 7.2

#### New "Overscale" command for scaling and aligning spectra

**Description**: A new scaling command has been added that makes it easier to compare spectra on a common scale when they have different baselines. The command is called "Overscale" and it is similar to doing "FullScale" followed by "CommonScale" and then manually dragging the spectra so their baselines coincide. The command can also be used to align peaks or midpoints. OverScale takes one argument that indicates what part of the spectra should be aligned as shown below.

"OverScale Baseline | Peak | Midpoint"

This command was added for the user interface of a new TQ Analyst version and is available as an OMNIC command because of a common codebase. It is not available through the OMNIC user interface yet.

#### History: This is an enhancement for 7.2

#### **Resolved Issues**

# OMNIC

# Correct diagnostic information displayed in OMNIC for a Nicolet 380 instrument

**Description**: The power supply diagnostics dialog available within OMNIC from the Diagnostic tab of Experiment setup now shows the correct list of voltages for a Nicolet<sup>TM</sup> 380 instrument. These voltages are for +5, +12, -12, +1.2, +2.5, +3.3 and -5 volts. In previous releases, only the +5, +12, -12 voltages were displayed. Also, the laser voltage readout has been removed from the Laser Diagnostics dialog when used with a 380 since the 380 does not provide this information. The laser voltage readout displayed for 380 instruments in previous releases was not accurate.

# History: This bug was introduced in OMNIC 7.1 when support was added for the Nicolet 380.

# Automatic atmospheric suppression available with Nicolet 380 instrument

**Description**: The checkbox for turning on automatic atmospheric suppression on the Collect tab of Experiment setup is now enabled when using a Nicolet 380 instrument. This allows users to perform automatic atmospheric suppression during data collect with a 380 instrument.

# History: This bug was introduced in OMNIC 7.1 when support was added for the Nicolet 380.

# Single-sided interferogram available with Nicolet 380 instrument

**Description**: The check box for specifying single-sided interferograms on the Advanced tab of Experiment setup is now enabled when using a Nicolet 380 instrument.

# History: This bug was introduced in OMNIC 7.1 when support was added for the Nicolet 380.

# Verify smart accessory available with Nicolet 380 instrument

**Description**: The button for verifying the Smart Accessory on the Diagnostic tab of Experiment Setup is now enabled when using a Nicolet 380 instrument.

# History: This bug was introduced in OMNIC 7.1 when support was added for the Nicolet 380.

# Saving spectra from Search results window

**Description**: Several menu items, including Save As, that were disabled when the Search result window was active are now enabled. This allows the Search Result window to be saved as a .WMF file.

#### History: This bug was introduced in OMNIC 7.0.

# Search and QC Compare from Macros Basic do not require user action to proceed

**Description**: OMNIC now correctly supports the Macros\Basic<sup>TM</sup> feature that allows Search and QC compare operations to complete and leave their result window open while the macro continues with no user interaction. In 7.0 and 7.1, the macro would not continue until the user manually closed the Search or QC Compare window.

# History: This bug was introduced in OMNIC 7.0.

#### Report fields not displayed when editing templates fixed

**Description**: In some situations, report fields were not being displayed when a template was edited. This would only happen if report fields were added and deleted in a specific order. This is now fixed.

# History: This bug has existed in all versions of OMNIC since 3.0.

# Autosave filename in title dropping last character fixed

**Description**: When the feature that allows the title of collected spectra to include the autosave filename was used (see the Collect tab of the Options dialog), the last character of the autosave prefix was dropped from the title. So if the autosave prefix was set to "abcd" and the sequence of collects results in a file being autosaved as "abcd0123.spa", the title would include "abc0123.spa" rather than "abcd0123.spa". This has been fixed.

# History: This bug has existed in all versions of OMNIC since 4.0.

#### Spectra not scaled properly when read from GRAMS multifiles

**Description**: When the ability to read GRAMS multifiles was added, the first scale factor in the file was used to scale all spectra. This has been changed to the individual scale factors.

#### History: This bug was introduced in OMNIC 7.0.

#### Save Range changed when it should not have in Experiment Setup

**Description**: On the Bench tab of Experiment Setup, if one of the properties lists that affect the recommended save range, such as Source or Window Material, is dropped down and then collapsed without making a change, the save range would be reset to the recommended range. This has been changed so the save range is only reset to the recommended range if one of the properties is changed.

#### History: This bug was introduced in OMNIC 7.0.

# Recommended Save Range not including Window Material when Bench tab first displayed

**Description**: When the Bench tab of Experiment Setup is first displayed, the Window Material was not included in the calculation of the recommended save range. This has been fixed. If any of the properties affecting save range was changed, the recommended range was calculated properly in earlier versions.

# History: This bug was introduced in OMNIC 7.0.

#### Find Peaks deletes peak labels outside of the region it is applied to

**Description**: The Find Peaks command is supposed to delete all peak labels in the region it is applied to before it adds the new labels. In 7.0, this was enhanced to leave annotation that was created using the peak height and peak area tools even if they are in the Find Peaks region. This change introduced a bug where some peak labels outside of the Find Peaks region were deleted by mistake. This has been fixed.

# History: This bug was introduced in OMNIC 7.0.

#### Preview Collect controls appear in collect window after a resize or change focus

**Description**: When the preview collect feature is used and the collect has progressed past the preview, the Start Collection button used to finish preview mode reappears by mistake in place of the save controls whenever a resize or focus change occurs on the collect window. This has been fixed.

# History: This bug was introduced in OMNIC 4.0.

# DDE Initiate messages no longer destroy global atoms

**Description**: OMNIC no longer destroys the global atoms used during processing of DDE initiate messages. Although destroying these atoms is the correct protocol, some Visual Basic programs that process the same DDE initiate messages crash if OMNIC does this. This may only be a problem on some versions of Windows.

# History: This bug was introduced in OMNIC 7.0.

# **Correct Velocities now displayed for Nicolet 380**

**Description**: In some circumstances, the wrong list of available velocities would be shown in Experiment Setup when used with the Nicolet 380. Several of the slow velocities would be missing. This has been fixed.

# History: This bug was introduced in OMNIC 7.1 when support was added for the Nicolet 380.

# Nicolet 380 does not work with the Centaurus microscope

**Description**: The Nicolet 380 would not collect data from a Centaurµs<sup>™</sup> microscope. This has been fixed.

# History: This bug was introduced in OMNIC 7.1 when support was added for the Nicolet 380.

# Cannot set Low pass filter on Nicolet 8700

**Description**: The Low pass filter on the advanced tab of Experiment Setup was never enabled when used with a Nicolet 8700. This has been fixed.

# History: This bug was introduced in OMNIC 7.1 when support was added for the Nicolet 8700.

# External trigger with a Nicolet Series instrument only works the first time

**Description**: The external trigger option in Series software would only work the first time. This was fixed by a driver change.

# History: This bug was introduced in OMNIC 7.0.

# MACROS PRO

# Export command displays save dialog when it should not

**Description**: When OMNIC DS is installed and "Prevent Overwriting of files" and "Prevent changing directories when saving files" policies are turned off in Thermo Security Admin tool, the DDE Export command displays the "Save As" dialog even when the destination file does not yet exist. This has been fixed.

# History: This bug was introduced in OMNIC 6.2.

# OMNIC v7.1a

# Resolved Issues

OMNIC

# OMNIC unstable after leaving Bench tab of Experiment Setup

**Description**: In some cases, if the keyboard focus is on the Sample Compartment row of the property grid on the Bench tab of Experiment Setup when a switch to another tab is done (or the dialog is closed) OMNIC will become unstable and communications with the instrument may be unreliable. One symptom of this is a completely blank tab displayed in Experiment Setup. A work around for this problem is to always change the keyboard focus to some row other than the Sample Compartment before leaving the Bench tab. This problem has been fixed so the work around is no longer needed.

# History: This bug was introduced in OMNIC 7.0.

#### Detector changes when Sample Compartment list is viewed

**Description**: In some cases, when the Sample Compartment list is dropped down and then collapsed without making a change, OMNIC will change the selected detector. The change in detector may also cause other fields to change such as the velocity and save range. This problem has been fixed.

History: This problem has existed in versions of OMNIC at least back to 6.0.

OMNIC v7.1

#### New Features

#### OMNIC

#### Peak Resolve.

**Description**: A new Peak Resolve menu item is available in the Analyze menu. Peak Resolve models or fits a number of pure peaks to a complex set of overlapping peaks in a sample spectrum. A table of the pure peaks is produced that can be printed or copied to the clipboard.

# History: This is an enhancement for 7.1

# Faster Control of Nicolet Series Instruments.

**Description**: When controlling a Nicolet Series instrument, OMNIC is no longer required to wait for each motor movement to complete before initiating the next operation. OMNIC does still wait for all movements to complete before initiating data acquisition. This change results in faster startup and more responsive changes in Experiment setup.

# History: This is an enhancement for 7.1

# New default configuration file.

**Description**: The default configuration file for OMNIC has been changed. If you have changed your default.con file, the OMNIC 7.1 installer will not overwrite the modified file. The changes include putting the toolbar across the top, using a smaller font size for annotation and prompting for the sample title at the end of sample collects rather than the beginning.

# History: This is an enhancement for 7.1

# Support added to Nicolet Series and Nexus drivers for Continuum XL.

**Description**: The Nicolet Series and Nexus<sup>™</sup> bench drivers have been enhanced to support collecting data from the array detector of the Continuum<sup>™</sup> XL.

# History: This is an enhancement for 7.1

# Environment variables now allowed in Menu and Toolbar paths.

**Description**: Paths to executables and macros assigned to toolbar items or menu items can now contain environment variables. The variables will be expanded at the time the item is selected by the user. This allows configuration files to be created on one machine and run on another where the target files are in a different location, as long as an environment variable exists that specifies the location.

# History: This is an enhancement for 7.1

# JCAMP-DX Enhancements.

**Description**: Raman spectra saved to JCAMP are now labeled with the ##DATATYPE string of RAMAN SPECTRUM instead of INFRARED SPECTRUM as stated in the JCAMP specification. Also, the XUNITS field for Raman spectra is now set to 1/CM instead of being left blank. The X and Y-axis units can now be set properly when Raman spectra saved with these enhancements are read back in.

As a separate issue, JCAMP files with YUNITS of TRANSFLECTANCE and now recognized and treated as Transmission spectra.

# History: This is an enhancement for 7.1

#### More pre-peak data points used for Raman collect above 4 cm-1 resolution.

**Description**: Previous versions used an interferogram peak position of 1024 when Raman collects were done at resolution of 2 cm-1 and higher. This has been changed to use the maximum number of pre-peak data points (usually 8192) at these higher resolutions. Testing has shown this improves the actual achieved resolution of some Raman collects.

# History: This is an enhancement for 7.1

#### Array Automation

#### Added ability to skip wells.

**Description:** In the Array Collect window, if preview mode has been selected for the collection, a button labeled "Skip well" will be displayed during the preview collects. If it is selected, the preview collects will stop and the data collection in the current well will be skipped. I.e., it will be as if the well had never been selected in the Wells tab.

# History: This is an enhancement for 7.1.

#### Improvements to the Array: Open Data Set window.

**Description:** There are several new capabilities in the Array: Open Data Set window related to the display of more than one spectrum in the window at the bottom.

If the shift key is held down while a well (or section of an expanded well) is left clicked, the spectrum will be added to the window at the bottom instead of replacing the one that is there.

If a row letter or column number is left clicked, all of the spectra from all of the wells in the row or column will be added to the window.

Multiple spectra can be selected or deselected in the window by clicking on the spectra with the Ctrl key held down (as in an OMNIC window).

The Select All and Clear items in the Edit menu are active as are the corresponding <Ctrl/W> and <Ctrl/Delete> accelerators.

The Full Scale, Common Scale, Offset Scale, and Display Limits items in the View menu are active, and operate on the spectra in the Array: Open Data Set window.

All selected spectra are copied to the selected OMNIC window by the Add button.

# History: These are enhancements for 7.1.

# Change well selection using arrow keys.

**Description:** In the Array: Open Data Set window (and the Collect Array window when the display is not in the "Live" mode), a well may be selected (for display) adjacent to the currently selected/displayed well by using the arrow keys to move to the well that is to the left or right of or above or below the current well.

# History: This is an enhancement for 7.1.

# Quant report allows All choice.

**Description:** In the Reprocess controls in the Array: Open Data Set window, if a quant method is selected as the metric and the Result has more than one Type defined in the quant method (e.g., several components in a CLS quant method), the Type dropdown list box will contain an additional choice: "All". If "All" is selected, when the Report button is selected, the spectra in the data set will be reanalyzed and the resulting \*.csv report file will contain separate columns for each of the components in the method.

# History: This is an enhancement for 7.1.

# Region controls provided for specifying correlation region.

**Description:** The Correlation option in the Reprocess controls in the Array: Open Data Set window has been modified as follows. If Correlation is selected as the metric, the **Region** edit controls are displayed allowing specification of a region of the spectrum that is to be used for the correlation operation. (Previously the entire spectrum was used.) The region tool is active to select the region graphically from the displayed spectrum.

# History: This is an enhancement for 7.1.

# Peak height ratio and Peak area ratio metrics available in reprocess.

**Description:** The Metrics available in the Reprocess controls in the Array: Open Data Set window now include "Peak height ratio" and "Peak area ratio". If either of these is selected, two radio buttons labeled "Numerator" and "Denominator" are displayed. When the former is selected, the peak or region and baseline edit controls are used to specify the frequencies of the peak or region and baseline to be used for the numerator of the ratio. The latter radio button allows specification of these frequencies for the denominator of the ratio.

# History: This is an enhancement for 7.1.

# Kinetics.

**Description**: A Kinetics Setup button has been added to the Methods tab of Array Setup that, if selected, displays a Kinetics Setup dialog. This dialog allows the user to specify how frequently the entire plate is to be measured and how many times it is to be measured.

# History: This is an enhancement for 7.1.

# New Array menu items.

**Description**: The Array menu has been expanded to include several new items that are active when an Array: Open Data Set window is displayed.

If the Show Array Information item is selected, a Collection and Processing Information window is displayed containing these data for the data set.

If the Change Title item is selected, the current title of the data set is displayed in a dialog and a new title can be entered.

If the Save Array As item is selected, a Save As dialog is displayed, allowing specification of a new file name into which a copy of the current data set will be saved. (This is useful if the Apply Function operation is to be done on a data set, and the original data need to be retained.)

If the Apply Function item is selected, a dialog is displayed allowing selection of a function to be applied to the spectra in the data set. Depending on the function selected, one or more other controls may appear in the window to specify the parameters for the function. E.g., if Smooth is selected, the number of smooth points must be entered.

If the Split Array item is selected, a dialog is displayed allowing selection of a range of wells whose spectra will be extracted from the current data set and stored in separately named .spa files.

# History: These are enhancements for 7.1.

# MACROS PRO

# Replaceable collect prompts.

**Description:** Two new strings have been added that control the text displayed in the prepare for sample and prepare for background dialogs that appear during data collects. The new DDE parameters are "Custom SamplePrompt" and "Custom BackgroundPrompt". The same settings are used for Raman and IR. Set the strings to the empty string to revert to the default prompts.

# History: This is an enhancement for 7.1.

# Interferogram peak level readable from Nicolet Series instruments.

**Description:** The new DDE parameter "BenchStatus InterferogramLevel" can be used to read the current interferogram level of a Nicolet Series instrument. This is available when data collect is active or inactive. The data is returned in the format

# History: This is an enhancement for 7.1.

# Environment variables supported in run commands

**Description:** The DDE commands Run, RunMacro, and RunMacroAndWait now allow Environment variables to be used to specify the location of the target. For example, the command [RunMacro "%OMNICDATA%\macro\SimpleTrans.mac"] will launch the SimpleTrans.mac macro from the macro subdirectory of the location set in the OMNICDATA environment variable. Note that OMNICDATA is set by the OMNIC installer and is normally set to C:\My Documents\OMNIC unless the user chooses to install to a different location. Other environment variables can be used as well as long as they have been initialized prior to the DDE command.

History: This is an enhancement for 7.1.

#### OMNIC DS

#### Administrator program requires username and password at startup.

**Description:** The Thermo Administration program now requires user authentication when the program starts to verify the user identity matches the user that is logged on to Windows.

#### History: This is an enhancement for 7.1.

#### Administrator program handles large networks better.

**Description:** The Thermo Administration program will switch to initiating the accounts on the local PC, rather than the accounts on the login domain if the enumeration takes a long time. An edit control has been added that allows user names to be entered manually so enumeration can be avoided. Accounts are not re-enumerated when switching from the access control portion of the tree to the policy portion.

#### History: This is an enhancement for 7.1.

# Administrator program more easily adds or removes access control entries for all access control functions.

**Description:** The Thermo Administration program has two new menu items. The "Add to All Access Control Items..." will add an Allow or Deny entry for the specified user to every function in the Access Control section of the application. The "Add to All Access Control Items..." will add an Allow or Deny entry for the specified user to every function in the Access Control section of the specified user to every function in the Access Control section of the specified user to every function in the Access Control section of the current application. The "Remove From All Access Control Items..." will remove the entry for a specified user or group from all functions in the Access Control section of the current application.

#### History: This is an enhancement for 7.1.

# Support for signing Libraries.

**Description:** Spectral libraries can now be signed using the new Sign button in Library Manager. The signature status of the selected library is shown at the bottom of the Library Manager Window.

# History: This is an enhancement for 7.1.

# Support for signing spectral group files (.spg).

**Description:** Spectral group files can now be signed and verified using the Sign File and Verify File items in the File menu.

History: This is an enhancement for 7.1.

#### Sign multiple files with a single authentication prompt

**Description:** The Sign File item in the File menu now allows multiple files to be selected for signing. The authentication prompt used to enter the password and signature reason is only displayed once and the same reason for signing is applied to all files.

# History: This is an enhancement for 7.1.

# Sign the selected spectra without using a file navigation dialog.

**Description:** A new item in the File menu called Sign Spectra will sign the selected spectra. If the spectra already have a filename associated with them, the file navigation dialog does not need to be displayed.

History: This is an enhancement for 7.1.

# Atlµs v7.1

The Atlµs<sup>™</sup> product has been completely revised. See the product documentation for information on changes to Atlµs.

#### Support for Nicolet Series Bench

Description: The Nicolet Series Bench drivers now support the Continuµm™ XL.

History: This is an enhancement for 7.1.

# **Resolved Issues**

#### OMNIC

#### Company Name change

**Description:** The company name has been changed from "Thermo Nicolet" to "Thermo Electron" in many places, such as copyright notices of help files and readme files.

History: This issue occurred in OMNIC 7.0.

# Current Tool changed after running a Macros Basic macro

**Description:** The selected tool may be changed incorrectly after running a Macros Basic macro.

History: This issue occurred in OMNIC 7.0.

# Spectrum title corrupted by Automatic Baseline Correct.

**Description:** A bug that caused the spectrum title to be corrupted when Automatic Baseline Correct was done has been fixed. This only happened if the title was at maximum length when the function was applied.

History: Problem introduced in 7.0.

#### Asterisk appended to spectrum filename

**Description:** When spectra were saved using the Save As dialog and the "Save as type" was set to show all files, an asterisk would be appended to the filename entered by the user. This has been fixed so nothing is appended to the filename.

**History:** Problem introduced in 7.0.

#### X Axis not drawn at start of data collect

**Description:** At the start of Collect Sample or Collect Raman, the X Axis would sometimes be left blank until a spectrum was added to the window. This drawing problem has been fixed.

**History:** Problem introduced in 6.0.

# X Axis always in decreasing order in Collect Window

**Description:** The X Axis in the Collect Window was always displayed in decreasing order. This has been changed to display the axis in the same order that the default limits are specified in the Window tab of the Options dialog.

History: Problem introduced in 6.0.

# X Axis limits changed at end of Raman collect

**Description:** When a Raman collect completed and the collected spectrum was added to a window, the X Axis of the window was reset to the zoomed out limits of the collected spectrum (always in decreasing order) and the default X Axis limits for new windows in the options were changed to these same values. All of this behavior has been removed so that adding spectra to a window at the end of a Raman collect behaves the same as all other methods of adding a spectrum to a window.

History: Problem occurred at least as far back as OMNIC 4.

# Multiple copies of Spectral Group files sent with Mail Spectra

**Description:** If more than one spectrum from the same .spg file were sent in the same email suing the Mail Spectra menu item, multiple copies of the .spg file were included in the email. This has been fixed so that only a single copy of the group file is attached.

**History:** Problem introduced in 7.0.

#### Collection and Processing Window garbled after closing spectral window

**Description:** If a Collection and Processing Information (CPI) window was left open after the spectral window it originated from was closed, some of the fields of the CPI window would become garbled. This has been fixed.

History: Problem in all previous versions of OMNIC.

# Interferogram peak not in display window of Experiment Setup

**Description:** In the bench tab of Experiment setup, if the save range was changed such that sample spacing had to change, the limits of the interferogram window were not adjusted correctly so the new peak position was within the displayed window. This has been fixed.

History: Problem introduced in 7.0.

# Overlay feature of Search results does not work when decimal point is a comma

**Description:** When Windows is set to use a comma as the decimal point, which is the default for some locales such as German, the overlay feature in the search results window did not work. This has been fixed, as well as problems with changing the number of search results using the Modify Display button.

**History:** Problem introduced in 7.0.

#### Use Fixed Scale during data collect not applied to interferogram collects

**Description:** The "Use fix Y-Axis limits in collect window" feature did not work when the final format of the collect was set to interferogram. This has been fixed, but the feature still does not apply to singlebeam collects so that background collects are not displayed using the limits intended for samples. Also, an error message is now displayed if the upper and lower values are set to the same value.

History: Problem introduced in 7.0.

# Buttons at bottom of Experiment Setup and Options cutoff when large fonts are used

**Description:** The buttons at the bottom of the Experiment Setup and Options dialog were cutoff when large fonts were used for the dialog caption. Selecting one of the Appearance Schemes from the Windows Display Properties dialog can set this large font. This has been fixed.

History: Problem introduced in 7.0.

#### **Dialog font intermittently incorrect**

**Description:** When the OMNIC dialog font was changed using the Options dialog, some dialogs would intermittently use the system font instead. This has been fixed.

**History:** Problem introduced in 6.0.

#### Extended Search text fields too short

**Description:** The text fields on the Extended Search tab of Library Setup were incorrectly limited to around twelve characters (depending on font size). The dialog now allows scrolling and uses the first 60 characters entered into these fields.

History: Problem occurred at least as far back as 5.2.

#### Green check appears before bench communications established

**Description:** With Nexus and Magna instruments, the green check indicating good bench status may appear before bench communications had been established. In this case, the green check appears, but the items in the collect menu remain disabled. This has been fixed.

History: Problem introduced in 6.2.

# Loading an old (pre 7.0) experiment file does not reset new fields

**Description:** If an experiment file created with a version of OMNIC prior to 7.0 is loaded, the new fields added in 7.0 are not reset to their default values. These fields include the auto-blank regions, the separate number of background scans and the Y-axis limits used during data collect. This has been changed so the fields added for 7.0 are reset to their default values so the older experiment files give the same behavior they did when they were created.

History: Problem introduced in 7.0.

# Problems with beamsplitter recognition on Nicolet Series instruments

**Description:** Problems on Nicolet Series instruments with the wrong beamsplitter being recognized as installed after an experiment file has been loaded have been fixed.

History: Problem introduced in 7.0.

# OMNIC DS

#### Editing annotation in the Annotation Information dialog corrupts signature status display.

**Description:** When annotation from a signed spectrum is editing using the Annotation Information dialog (available from the Collection and Processing Information window), the displayed signature status of the spectrum with change to the string "Text". This has been fixed.

History: Problem introduced in 7.0.

#### **Known Issues**

# Tabbing in Options and Experiment Setup does not move between controls.

**Description:** Pressing the tab key does not move the keyboard focus from one control to the next in the Options and Experiment Setup dialogs.

**Recommendation:** Use the mouse to move keyboard focus to a control.

**History:** Problem occurred in all previous versions.

# Inserting a smart accessory during a data collect.

**Description:** On a Nicolet series instrument, if a smart accessory is installed while a data collect is active, the experiment file will be changed in the middle of the collect, possibly resulting in bad scans. Other instrument types suppress the change if a data collect is active. However, if an accessory is inserted while the collect is active, the IR beam will almost certainly be disrupted resulting in bad scans anyway.

Recommendation: Accessories should not be changed during data collect.

History: Problem introduced in 7.0.

# OMNIC v7.0

# New Features

# OMNIC

# Anti-collision for annotations in Find Peaks.

**Description**: The Find Peaks operation in OMNIC now adjusts the location of peak labels to avoid overlapping labels as much as possible.

# History: This is an enhancement for 7.0

# Support for Nicolet Series instruments.

**Description**: Support for the Nicolet Series line of instruments is now included. This includes providing control for filter wheels, screen wheel, polarizer, turbo source, and function buttons on the front of the instrument.

# History: This is an enhancement for 7.0

# Grid of controls used on Bench tab of Experiment Setup.

**Description**: The controls on the bench tab of the Experiment Setup dialog have been consolidated into a grid to reduce clutter, make better use of space and handle dynamic bench configurations better. This required a few other small changes to the layout of the Bench tab.

# History: This is an enhancement for 7.0

# Freeze button on Bench and Diagnostic tabs of Experiment Setup.

**Description**: A "Freeze" button has been added to the bench and diagnostic tabs of Experiment setup that will snapshot the currently displayed interferogram or singlebeam and leave is displayed in the window so it can be compared to subsequent scans.

# History: This is an enhancement for 7.0

# New Configure tab of Experiment Setup.

**Description**: A Configure tab has been added to the Experiment Setup dialog. This tab has the "Configure Bench" button that was on the Diagnostics tab, along with controls for providing

names for the positions of the filter wheels and screen wheels (if they are present) and setting up the IR Source rest mode for instruments that support this feature. Items set up this tab are not saved in experiment files.

# History: This is an enhancement for 7.0

# X Limits of live display persist in Experiment Setup.

**Description**: The X limits of the live display are not saved when the dialog is closed and reused when you redisplay the dialog. The limits are also saved when you switch to between the Bench and Diagnostics tabs. The are not saved when you exit OMNIC.

# History: This is an enhancement for 7.0

#### Background scans optionally set separate from Sample scans.

**Description**: The Collect tab of experiment setup now provides an option to specify a different number of scans for the background than the sample.

# History: This is an enhancement for 7.0

# Option to set Y-Limits for use during collect.

**Description**: The Collect tab of Experiment Setup now provides an option to specify a Y limits to be used in the collect window during the collect operation. This can be used to avoid autoscaling on large peaks that are not of interest.

#### History: This is an enhancement for 7.0

#### Auto-blank regions during data collect.

**Description**: The Advanced tab of Experiment Setup now provides a grid for entering up to four spectral regions that are to be blanked during data collection. The regions can be turned on and off individually. This new auto-blanking feature can be used when collecting with accessories that have totally absorbing regions to prevent auto-scaling to these large peaks.

#### History: This is an enhancement for 7.0

# Marco assigned to front panel button on instrument.

**Description**: The Advanced tab of Experiment Setup now provides a place to identify a macro that will be executed when the "Macro" button on the front panel of the Nicolet Series instrument is pressed.

# History: This is an enhancement for 7.0

#### Improved peak annotations.

**Description**: The annotations created with the peak height and area tools now use lines or shading to highlight the measured peak.

# History: This is an enhancement for 7.0

#### Annotations viewable as a table.

**Description**: The annotations associated with a spectrum can now be viewed as a table by clicking the new "Annotations" button in the Collection and Processing Information window. The text portion of the annotation can be editing in this window, but the location and baseline information cannot. The table can be copied to the clipboard.

# History: This is an enhancement for 7.0

# Mail Spectra.

**Description**: A new Mail Spectra item in the File menu provides support for sending the currently selected spectra as attachments to an email message. The email is sent using the default account for the logged on user.

# History: This is an enhancement for 7.0

# Additional Y Scaling buttons.

**Description**: Two additional buttons are now provided in the View Finder control to improve scaling in the Y dimension.

# History: This is an enhancement for 7.0

# List of spectral titles auto-sizes.

**Description**: The drop down list of spectra at the top of the main spectral window is now sized so that empty rows are eliminated and do not obscure the spectra display.

# History: This is an enhancement for 7.0

# Additional techniques supported for Derivative.

**Description**: The Derivative operation on the process menu has been enhanced to three choices of techniques: 1) First different (the only technique supported in previous versions), 2) Savitzky-Golay and 3) Norris.

# History: This is an enhancement for 7.0

# Overlay spectra in Search Results window.

**Description**: The spectral display in the Search results window now can be switched between stack and overlay mode. This allows the unknown to be overlaid with one or more of the search hits.

# History: This is an enhancement for 7.0

# Multifile .SPC file read.

**Description**: OMNIC now read all of the spectra in GRAMS .SPC files that contain more than one spectrum.

# History: This is an enhancement for 7.0

# New look for tabbed dialogs.

**Description**: Some cosmetic changes were made to the look of the tabbed containers used for the Options dialog and Experiment Setup dialog.

# History: This is an enhancement for 7.0

# Saving spectra from Spectral Group files now defaults to saving as individual files.

**Description**: In earlier versions of OMNIC, when you read in spectra from a spectral group file (.spg) and then did a save with one of the spectra from the .spg file selected, the group file would be overwritten with a new group of just that one selected spectra. To avoid that problem, save operations on spectra that were loaded from .spg files default to saving as individual spectra in .spa files.

# History: This is an enhancement for 7.0

# Floating-point exceptions now handled more gracefully.

**Description:** Floating point exceptions that occur in OMNIC are now caught and acknowledged so that the application does not exit. For example, in earlier versions of OMNIC, you could enter very large numbers in the Spectral Math window and generate a floating-point exception that would cause OMNIC to exit. This error is now caught and handled properly.

#### History: This issue occurred in OMNIC DS version 6.2.

#### OMNIC DS

#### Administrator program translated.

**Description:** The Thermo Administration program is now translated into several languages.

#### History: This is an enhancement for 7.0.

#### Warning at OMNIC start for invalid directory policies.

**Description:** OMNIC now gives a warning at startup if any of the initial directory policies set in the Thermo Administration program are not valid. This is done at OMNIC startup rather than in the Thermo Administration program to handle cases where directories are deleted after the policies are set.

#### History: This is an enhancement for 7.0.

# SST and TRS

# Synch Hold Addition to SST

**Description:** A new option has been added to AM, PM, and TRSS step-scan collects. This is the ability to specify that the stepping be triggered externally rather than occurring automatically after the data collection. This external trigger should be connected to the bench via the SYNCH BNC. If this feature is enabled, and the logic level on this input is high after the data collection, the stepping to the next mirror position will be delayed until the level goes low. This option is available only if the firmware is version 7.16 or later

#### History: This is an enhancement for 7.0.

#### **Resolved Issues**

#### OMNIC

#### Collect time-out when set to ssp1 @ .125 cm-1 resolution with PCI card

**Description:** When data is collected about 7879 cm-1 at .125 resolution, data collect timeouts could occur. Only occurred on Magna or Nexus instruments that used a PCI interface card. This has been fixed.

#### History: This issue occurred in OMNIC version 6.1 and 6.1a.

#### Problems showing data in increasing X order fixed.

**Description:** If the X-Limits were set so the left limit was less than the right limit (increasing order), a bug caused OMNIC to switch the order back to decreasing when the View Finder control was touched. This appeared in the Bench tab of Experiment setup and could also occur in the main spectral window if the limits were manually set.

# History: This issue occurred in OMNIC version 6.2 and earlier.

# File types recorded separately for Open and Delete file dialogs.

**Description:** The Open and Delete file dialogs use to share a setting to record the last file type the user selected so that type could be selected again the next time the dialog was shown. This gave unexpected results because the list of file types in the two dialogs is not the same. There are now two separate settings to record the last file type so the open and delete dialogs each remember the last selection correctly.

# History: This issue occurred in OMNIC version 6.2 and earlier.

# Filename now shows when bitmap pasted into external program.

**Description:** If the filename field of Sampling information is turned on when a copy is done of the spectral window and pasted into an external program such as Microsoft Word, the filename was not shown in the pasted image. This has been fixed.

# History: This issue occurred in OMNIC version 6.2 and earlier.

# Mpanel32.exe no longer installed.

**Description:** The Mpanel32.exe program provided a way to launch Macros Basic macros in the original versions of OMNIC that did not have a toolbar (versions 1 and 2). Since macros can now be assigned to the toolbar, this program is no longer needed so it has been removed from the install.

# History: This issue occurred in OMNIC version 6.2 and earlier.

# Collection and Bench parameters saved in new user libraries for each spectrum.

**Description:** A limitation of user libraries has been eliminated for new libraries created with OMNIC 7. When a spectrum is extracted from a user library, the true collection and bench parameters of that were used to collect the spectrum are now retrieved from the library rather than the ones from the first spectrum in the library. If the spectrum was deresolved or hyper-resolved as it was added to the library, looking at the sample spacing vs. the resolution can identify it. A warning will be displayed if a spectrum needs to be hyper-resolved when added to a library.

# History: This issue occurred in OMNIC version 6.2 and earlier.

# Spectrum filename can be displayed in Search window.

**Description:** The filename of the unknown spectrum now displays properly in the Search window when the display setup has this feature turned on.

# History: This issue occurred in OMNIC version 6.2 and earlier.

# Improved parsing of OMNIC command line.

**Description:** Improvements were made to the parsing of the OMNIC command line so that double clicking on files in Explorer with filenames that included dashes is now handled correctly.

History: This issue occurred in OMNIC DS version 6.2.

# Changes made to spectra extracted from report do not affect report display.

**Description:** A bug that caused the display of reports to be modified when changes were made to spectra extracted from the report has been fixed. The changes shown on the report display were never written to the report, but the display was mistakenly being modified.

# History: This issue occurred in OMNIC DS version 6.2.

# OMNIC DS

#### Saving data to protected directories works as installed.

**Description:** The feature of DS that allows users to save data into directories they would normally not have write permission on no longer requires administrators to manually change the permissions on each users temp directory. This bug has been fixed so that the feature works with the permissions set at install.

# History: This issue occurred in OMNIC DS version 6.2.

#### Problems signing files after password change on Windows XP fixed.

**Description:** A security feature of Windows XP invalidates the default PKI keys under some circumstances when a password change occurs. When XP service pack 1 is installed, this only occurs if the administrator forces a password change. Without service pack 1 installed, this can occur even when the user changes the password. After the default keys are invalidated, OMNIC will no longer be able to sign or verify files for that account. A change has been made in 7.0 so that OMNIC does not use the default keys and is therefore not affected by password changes.

#### History: This issue occurred in OMNIC DS version 6.2.

#### Print feature of Search window now uses printing policy correctly.

**Description:** The print feature of the Search results window is now disabled if the unknown spectrum has not been saved and the security policy is set to prevent printing of unsaved data.

#### History: This issue occurred in OMNIC DS version 6.2.

#### Spectra extracted from library can now be printed regardless of printing policy.

**Description:** The policy that controls printing of unsaved data was preventing spectra extracted from a user library from being printed. These spectra are now correctly marked as saved so they can be printed regardless of the policy setting.

#### History: This issue occurred in OMNIC DS version 6.2.

#### Windows key no long gives access to explorer features in open/save dialogs.

**Description:** The policy that prevents users from having access to the Explorer features such as delete and rename could be defeated in 6.2 by pressing the Windows key. This has been fixed so user cannot access Explorer functions.

#### History: This issue occurred in OMNIC DS version 6.2.

#### Event log entries now made for file deletions for GAML files.

**Description:** File delete entries were not being made when GAML files were deleted. These entries are now made, but the filename recorded for all delete operations is the 8.3 version, so they show up as deletions of .GAM files.

History: This issue occurred in OMNIC DS version 6.2.

OMNIC v6.2

New Features

OMNIC

# Read/Write GAML files.

**Description:** Added ability to read and write spectra in GAML format.

History: This is an enhancement for 6.2.

#### New Advanced ATR correction.

**Description:** Added New Advanced ATR correction.

History: This is an enhancement for 6.2.

#### Insertion and deletion date now available for library spectra.

**Description:** With libraries created in OMNIC 6.2, the insertion and deletion dates of each spectrum is tracked. The dates are visible in the Library Spectra tab of library manager. This information is not available for libraries created prior to 6.2, even when new spectra are added to these libraries.

#### History: This is an enhancement for 6.2.

#### Spectra deleted from user libraries remain visible until the library is compressed.

**Description:** A new column has been added to the Library names tab of Library Manager with the heading "Del". A red X in this column indicates that the spectrum has been deleted from the library. Compressing a library permanently removes the deleted spectrum from the library. After compression no red X's are displayed in the "Del" column.

#### History: This is an enhancement for 6.2.

#### Display help files in three-pane mode.

**Description:** Additional files are being installed so that help files will be displayed in the more modern three-pane mode.

#### History: This is an enhancement for 6.2.

# Resizing Open/Save dialogs.

**Description:** Several open/save dialogs where changed so they can be sized by the user. Also, small improvements were made in the spacing/alignment of controls on open/save dialogs.

#### History: This is an enhancement for 6.2.

# Remember size of Spectrum information window

**Description:** If the Spectrum information window is enlarged beyond it's default size, the new size is saved and used as the initial size for the window the next time it is opened.

# History: This is an enhancement for 6.2.

# Record old data spacing for Change Data Spacing

**Description:** The history entry made in the spectrum header when a Change Data Spacing operation is performed now includes the old data spacing as well as the new data spacing.

# History: This is an enhancement for 6.2.

# Raman operations generate history records.

**Description**: The Raman operations Shift, Un-shift and Instrument correct now generate records in the spectrum history.

# History: This is an enhancement for 6.2.

# Change Data Spacing history now includes old data spacing.

**Description**: The history record generated when a change data spacing operation is done now includes both the old and the new data spacing. Previous versions only record the new data spacing.

# History: This is an enhancement for 6.2.

# OMNIC DS

# Admin program for configuring user authorization.

**Description**: Authorization to use any OMNIC function now controlled by separate Administration program.

History: This is an enhancement for 6.2.

# Reasons for Digital Signatures controlled by Admin program.

**Description**: Access to reasons for signatures now controlled in the Admin app.

# History: This is an enhancement for 6.2.

# Event Log for significant events.

**Description:** Significant events such as saving data and signing files are recorded in an isolated section of the NT Event log. Modifications, deletions and renaming of important file types generate log events, even when they are made outside of OMNIC.

# History: This is an enhancement for 6.2.

# Saving data to directories with restricted access.

**Description:** Added ability to save files to directory that has very restricted access so lab manager be assured files will not be renamed or deleted. Even with this restricted access, OMNIC is able to apply digital signatures to the files.

# History: This is an enhancement for 6.2.

# Sign file gives three chances to enter correct password.

**Description:** The sign file dialog now gives the user three chances to enter the correct password.

# History: This is an enhancement for 6.2.

# SST and TRS

# **New Sample Spacing choices**

**Description:** Increased range of allowed sample spacings for step scan experiments from 8 to >100. (Requires bench firmware v. 7.14)

# History: This is an enhancement for 6.2.

# Improved multiple-trigger mode

**Description:** Improved multiple-trigger mode operation in TRSS collects by allowing shorter trigger intervals. (Requires Gage driver v. 3.60 or later)

#### History: This is an enhancement for 6.2.

# Resolution selection for step-scan time-resolve

**Description:** Made resolution selection more flexible for step-scan time-resolved collects.

#### History: This is an enhancement for 6.2.

#### Y-axis added to TRSS real-time display

**Description**: Y-axis added to TRSS real-time display.

#### History: This is an enhancement for 6.2.

#### Step-Scan Settling time now set with edit control

**Description**: The Settling time control in the Step-Scan Time-Resolved setup dialog has been changed from a list box to an edit control to allow more flexible setting of this parameter. The minimum value is 1 msec or larger if more time is required for data transfer during multiple-trigger collection.

#### History: This is an enhancement for 6.2.

#### **Resolved Issues**

# OMNIC

# Change the default setting for the Bench and Collect checkboxes to off in the Quant Setup dialog.

Description: Change in default behavior.

# History: This issue occurred in OMNIC version 6.1a and earlier.

# Change how the spectral limits in a new Raman library will be created.

**Description:** Correct a problem with frequency normalization whit Raman shifted data. This is now the correct behavior, but there will be a difference between old Raman libraries and new Raman libraries with respect to how the spectral limits are normalized.

# History: This issue occurred in OMNIC version 6.1a and earlier.

#### Change to not display an error when a user chooses not to overwrite a signed file.

**Description:** Eliminate an erroneous error message that was displayed when the used chooses not to overwrite a signed file.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

# Fixed a bug that occurred when OMNIC was installed in a path that used multi-byte Japanese characters.

**Description:** Fixed a bug that occurred when OMNIC was installed in a path that used multi-byte Japanese characters.

# History: This issue occurred in OMNIC version 6.1a and earlier.

# On a clean install, the default for peak picks will be sorted on Position, not intensity.

**Description:** On a clean install, the default for peak picks will be sorted on Position not intensity.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### Setting access rights to temporary directory.

**Description:** A change was made to set the users temporary directory to have wide-open access each time OMNIC starts. This allows ancillary OMNIC tools to write to this directory.

# History: This issue was not a problem in earlier versions of OMNIC.

#### Turn off display of signature information in reports.

**Description:** Changed the report printing to turn off display of signature information for spectra because spectra in reports are never signed. Only the notebook can be signed.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### Spectra from signed .spa files appear modified when loaded.

**Description:** Fixed a bug where spectra loaded from signed .spa files were considered modified as soon as they were read. This bug caused a prompt to resave the spectra when the window was closed, even though the spectra had not actually been modified.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### Change to allow up to 10000 series files in sequence rather then 100.

**Description:** The automatically generated filenames for series files now have enough digits to allow 10000 files in the same directory rather than 100.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### Cleanup drawing flaws in skinned dialogs.

**Description**: Some small improvements to the skinned drawing of dialogs were made, such as providing a background color to list boxes and using a solid brush color if pattern bitmaps are not available.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### Fixed a bug that would disable the spectrometer tour by mistake in some cases.

**Description**: Fixed a bug that would disable the spectrometer tour by mistake in some cases.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### MRU list saved on a per-user basis.

**Description**: The MRU list of spectra at the end of the File menu is now stored in the registry on a per-user basis rather than in Omnic32.ini. The main reason for this change is that some user sites prefer to set all files in the Windows directory (including Omnic32.ini) as read-only for standard users. When this is done, OMNIC's MRU list would not work.

# History: This issue occurred in OMNIC version 6.1a and earlier.

# OMNIC sub-installers have been changed to use Microsoft Installer.

**Description**: Many of the OMNIC sub-installers have been changed to use the new Microsoft Installer technology. This was done for improved maintainability since the old InstallShield installer is no longer supported.

# History: This change was made to avoid future problems.

#### Spikes in files converted from Perkin Elmer format fixed.

**Description**: Fixed the Perkin Elmer spectral conversion code so that it does not produce spikes when data values are near zero.

# History: This issue occurred in OMNIC version 6.1a and earlier.

#### Undo Scale must be done twice.

**Description**: A bug that required Undo Scale Change to be done twice to undo changes made with the zoom buttons of the view finder was fixed.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### Raman Instrument correct works with a reference file.

**Description**: A bug that prevented using a reference file for Raman Instrument Correct was fixed.

#### History: This issue occurred in OMNIC version 6.0, 6.1 and 6.1a.

#### Options changes recognized in Find Peaks window.

**Description**: Find Peaks windows now recognize changes to options such as annotation orientation and number of digits. Earlier versions required the Find Peaks window to be closed and reopened for the change to take effect.

# History: This issue occurred in OMNIC version 6.1a and earlier.

#### Drawing shaded regions on 32 bit depth ATI cards changed.

**Description**: A different technique is now used to draw shaded regions. The old technique did not work on some ATI cards when the bit depth was set to 32 bits.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### Additional message generated if file signing canceled.

**Description**: If a user is required to sign a file as part of the save operation, but cancels the signature dialog or enters an invalid password 3 times, an error message is now displayed indicating the file has been saved, but not signed.

# History: This issue occurred in OMNIC version 6.0, 6.1, and 6.1a.

#### References to Thermo web site changed.

**Description**: The references to the Thermo Electron web site have been changed to www.thermo.com/Spectroscopy.

#### History: This issue occurred in OMNIC version 6.0, 6.1, and 6.1a.

# Crash when invalid gain read from a file.

**Description**: A bug that caused a crash when an invalid gain was read from a spectrum file was fixed.

# History: This issue occurred in OMNIC versions 6.1, and 6.1a.

#### More scans button on collect window disabled for Mattson.

**Description**: A problem adding additional scans after a data collect was initiated on Mattson benches was fixed by disabling the feature when OMNIC is running with one of these benches.

# History: This issue occurred in OMNIC versions 6.1, and 6.1a.

#### Failure to overwrite read-only configuration files now reported.

**Description**: Attempting to save over the top of a read-only configuration file now generates an error message indicating the save failed. In prior versions, the save failed with no indication.

# History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Failure of Change data spacing now reported.

**Description**: When the Change data spacing command fails, an error message is displayed. Attempting to change the data spacing of an interferogram is an example of how the command can fail.

#### History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Hourglass cursor now shown during Other Conversions.

**Description**: The hour glass cursor is now displayed during the other conversions command since some of these conversions can be time consuming.

#### History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Digital Signature status not shown properly for Almega spectra

**Description**: A bug that prevented the digital signature status from being displayed for Almega spectra was fixed.

#### History: This issue occurred in OMNIC versions 6.0, 6.1, and 6.1a.

#### Text drawing bug in collect status window fixed

**Description**: A bug that caused several text strings to be drawn on top of one another in the collect status window was fixed. This occurred if the experiment description and title were blank.

#### History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Spectra filename lost after an undo operation fixed

**Description**: If an operation is performed on a spectrum that had been saved to a file and then the operation undone, the spectrum would appear as if it had never been saved to a file and the user would have to re-assign a filename. This is now fixed.

#### History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Crash when adding very long annotation fixed

**Description**: If a piece of annotation was added with a very long text string (2000 characters), a crash could occur. This has been fixed by checking for a maximum buffer size.

# History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Remove DC offset from interferograms read from Mattson files.

**Description**: A correction is now done to remove the DC offset from interferograms read from Mattson files before the data is displayed or processed.

# History: This issue occurred in OMNIC versions 6.0, 6.1, and 6.1a.

#### Normalize Scale command failed when performed twice.

**Description**: A problem was fixed with the Normalize Scale command. If the command was performed twice on the same spectrum the results were invalid. On some PC's a floating-point exception was generated and OMNIC would exit.

#### History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Change to the default value in Quant setup.

**Description**: In the Quant Setup dialog, the default setting for the Bench and Collect check boxes was changed from on to off.

#### History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Raman data added to library had poorly registered X-axis values.

**Description**: When a Raman spectrum was added to a library the x-axis values were not properly registered to the laser frequency. This problem is now corrected.

#### History: This issue occurred in OMNIC versions 6.1a and earlier.

#### Initial directory for Configuration files is now the same as parameter files

**Description:** The initial directory for configuration files was changed to be the same as the initial directory for parameter files instead of options.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### **GC-FTIR External trigger feature fixed**

**Description:** A problem where a Series GC collect waiting for an external trigger from the GC device would start before the trigger signal was issued was fixed.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

# SST and TRS

# Display of Channel B/A ratio in PEM setup dialog

**Description:** Fixed bug in display of Channel B/A ratio in PEM setup dialog.

#### History: This issue occurred in OMNIC version 6.1a and earlier.

#### Collect time-out problem in step-scan dialogs.

**Description:** Fixed collect time-out problem in step-scan setup dialogs when averaging time is large (> 3 sec).

#### History: This issue occurred in OMNIC version 6.1a and earlier.

# Phase Analysis dialog.

**Description:** Modified Phase Analysis dialog so that IP spectrum must be in upper window.

# History: This issue occurred in OMNIC version 6.1a and earlier.

# SST menu item names.

Description: Changed SST menu item names and labels for several controls in setup dialogs.

# History: This issue occurred in OMNIC version 6.1a and earlier.

# OMNIC v6.1a

# **Resolved Issues**

# OMNIC

# The new GMT time zone information in the Data Display Information section of the Spectral History is displayed improperly when on the positive side of the grand meridian.

**Description:** The title contains the correct time stamp (Mon Jul 29 14:39:05 2002 (GMT+02:00)), but DS date and time in the spectral header says " 29-07-2002 15:40:36 (GMT-11330037:44)".

History: This issue occurred in OMNIC version 6.1. Tracking number: V&V3677.

# Changed the Spectrometer Tour routine to not check the CDROM drive for the tour.

**Description:** This fixes a message (abort, ignore, retry) that pops up on some computers and OS combinations when a CDROM is not in the drive.

History: This issue occurred in OMNIC version 6.1.

# Rapid scan collects stalled on Windows NT 4.0 systems.

**Description:** Rapid scan was not functioning properly on Windows NT<sup>®</sup> 4.0 systems.

History: This issue occurred in OMNIC version 6.1 driver. Tracking number: V&V3693.

# Intermittent driver problem could result in a system lockup during data collect.

**Description:** This issue was discovered during internal testing. Rapid scan was not functioning properly on Windows NT 4.0 systems.

History: This issue occurred in OMNIC version 6.1 driver.

# InterpretIR+

# InterpretIR+ did not install from the Update CD.

**Description:** InterpretIR+<sup>TM</sup> did not update the previous version since the name of the executable had changed. This has been corrected.

History: This issue occurred in OMNIC version 6.1 Update CD.

# Val-Q

# Some Autotest results report failures when run under some foreign languages.

**Description:** The references used in the comparison were created on a system where decimals are used as the numerical separator. Changed software testing module in Val-Q to recognize commas in place of decimals as valid separators.

History: This issue occurred in OMNIC version 6.0a.

# Autotest report four failures when run on a system that does not have the DS option installed.

**Description:** Autotest was reporting failures because it cannot read the digital signature portion of a data file without having the DS option installed. Autotest changed to perform the correct comparison with and without the DS option.

History: This issue occurred in OMNIC version 6.1 driver.

# **View Stage**

# Cannot view data during data collection.

**Description:** Changed FT Raman software to not turn off the Raman View Stage lamp when collecting data since the lamp LED does not affect Raman data. This allows you to view data while collecting.

History: This issue occurred in OMNIC version 6.1.

# Almega

# Photobleaching not operating properly.

Description: Correction to PolySNR test which caused photobleaching to be done twice.

History: This issue occurred in OMNIC for Almega version 6.1.

# Slit selection changing when switching tabs.

**Description:** The 10 um slit option did not remain selected when changing tabs.

History: This issue occurred in OMNIC for Almega version 6.1. Tracking number: V&V3634.

# Display limits when viewing data in nanometers..

**Description:** Display limits for preview data collect were incorrect when final format is in nanometers.

History: This issue occurred in OMNIC for Almega version 6.1. Tracking number: V&V3635.

# Updating previous Almega installations with the Update CD.

**Description:** The Almega driver did not update when installed from the Update CD. This has been corrected. Does not affect new installations.

**History:** This issue occurred in OMNIC for Almega version 6.1.

# SST and TRS

# PM setup dialog and multiple frequency selection.

**Description:** Changes and bug fix in PM Setup dialog related to multiple frequency selection and use.

**History:** This issue occurred in OMNIC version 6.1.

# Autogain limits and trigger intervals.

**Description:** Changed the lower limit from 4.5 to 4.0 volts in autogain checking. Also upped the minimum trigger interval from 0.01 sec to 0.04 sec. **History:** This issue occurred in OMNIC version 6.1.

Thermo Scientific Page 69 of 85

# OMNIC v6.1

# **New Features**

Brief descriptions of the new features in OMNIC version 6.1 software suite are provided below.

# Added EZ OMNIC support for IR100 and IR200 spectrometers. Add diode laser capabilities and verification for the IR100 and IR200 spectrometer to EZ OMNIC.

**Description:** The IR100 and IR200 Series FT-IR spectrometers were designed to meet the needs for fundamental infrared analysis, teaching and basic sampling needs. The IR100 and IR200 spectrometers also operate with the Encompass<sup>TM</sup> software. EZ OMNIC support is now provided for those customers that prefer the flexibility of a personal computer with more functionality.

History: Feature added to EZ OMNIC v6.1

# Added support for ECO 3000 FT-IR spectrometer.

**Description:** The ECO<sup>TM</sup> 3000 is a 300 mm, high-performance, tool used for measuring dopant levels in dielectric films (BPSG, PSG, FSG), Hydrogen in SiN/SiON films, epitaxial film thickness, MEMS device thickness, and Carbon and Oxygen in Silicon wafers. The ECO 3000 supports the SEMI standards for 300mm automated wafer handling.

History: Feature added to OMNIC v6.1

# Added support for Avatar 330 and 370 spectrometers.

**Description:** The Avatar<sup>™</sup> 330 and 370 spectrometers are routine analysis FT-IR spectrometers that offer packaged solutions for your entire FT-IR process, from data collection to reporting the results.

History: Feature added to OMNIC v6.1

# Added support for Windows XP Professional and Home Editions.

**Description:** Support for Windows XP version is available in this release. Windows XP Professional is required with the Digital Signature (DS) option.

History: Feature added to OMNIC v6.1

# Added the capability to change the font used in all dialog boxes of OMNIC in the Edit/Options/View tab.

**Description:** This improves the legibility in the dialogs when fonts for a specific region such as in Czechoslovakia or a bolder font is used.

History: Feature added to OMNIC and EZ OMNIC v6.1

# Added a (GMT-6:00) string to display time zone in the date/time strings used for digital signatures.

**Description:** The FDA recently released a guidance document regarding time stamp requirements for Part 11 of Title 21 of the Code of Federal Regulations. To aid in a clear understanding of the time zone in which an event occurred, a reference to GMT is appended to each record of the time written into the Collection and Processing Information.

History: Feature added to OMNIC v6.1.

# Added the capability to digitally sign Macros\Basic (.MAC) file in OMNIC.

**Description:** Macros files play a key role in a system that is subject to the FDA's 21 CFR Part 11 regulations as they can be used to enforce permitted sequencing of steps and events. By using the Sign File command in the OMNIC File menu, users can sign these files and later verify the a macro has a valid digital signature with the Verify File command in the File menu.

History: Feature added to OMNIC v6.1

# Removed the checkbox for signing group files in the Edit/Options/Security tab. Also, spectral groups are not listed as a file type in the Sign File dialog.

**Description:** The ability to sign group files was confusing to some users. A group file consisted of a group of spectra, stored together in a single file. User's were confused as to the meaning of the signature on the file and how it related to the individual spectra in the group file.

History: Feature added to OMNIC v6.1

# When copying a report to the clipboard, the report is placed in the clipboard as a bitmap as well as a metafile.

**Description:** Users now have the option to copy and then paste reports from a report notebook into another application as either a bitmap or a Windows metafile.

History: Feature added to OMNIC v6.1

# Added new 'GetBenchName' DDE routine. It gets the bench name and puts it into result current.

**Description:** Users can query the spectrometer for its model name. The complete command line for this option is described in the Macros on-line help file.

History: Feature added to Macros Basic v6.1 and Macros Pro v6.1.

# Added new Delay DDE command. It can be used in a macro to delay for a specified number of seconds.

**Description:** If a user created a macro where one event must wait for another to complete, the user can add a delay into their macro for a specified number of seconds. The complete command line for this option is described in the Macros on-line help file.

History: Feature added to Macros Basic v6.1 and Macros Pro v6.1.

# Enabled the "Other Conversions" menu command in the Process menu of EZ OMNIC.

**Description:** The Other Conversions command that previously was available only in OMNIC, now appears in the EZ OMNIC menu. Other conversions allow the user to convert a spectrum into Kubelka-Munk, Photoacoustic, %Reflectance, Log (1/R), wavenumber, micrometers or nanometers.

**History:** Feature added to EZ OMNIC v6.1

#### Improved Issues

# Substantially decreased the amount of time to start OMNIC for Nexus and Avatar series spectrometers.

**Improvement:** When OMNIC is started, the user can now access the OMNIC menus more quickly without having to wait until the spectrometer setup has been completed. Note that the OMNIC data collection menu items and the bench status indicator will not be enabled until the spectrometer setup is complete.

**History:** This issue occurred in OMNIC versions 4 through 6.0a. Tracking number: ENH03346.

# Substantially decreased the amount of time to start OMNIC when using the Digital Signature (DS) option on a computer that is not physically connected to a network.

**Improvement:** When OMNIC is started, the user can now access the OMNIC menus more quickly without having to wait until the spectrometer setup has been completed. Note that the

OMNIC data collection menu items and the bench status indicator will not be enabled until the spectrometer setup is complete.

History: This issue occurred in OMNIC version 6.0a Tracking number: N/A.

# Added capability to capture the user name with every modification that is recorded in Collection and Processing Information.

**Improvement:** If the Digital Signature option is installed, OMNIC users are required to enter their Windows NT, Windows 2000 or Windows XP username and password to start OMNIC. The full user name along with the date-time is recorded in the Collection and Processing Information whenever data is collected, modified or signed. Similarly, if a user does not have the DS option but has enabled the OMNIC login feature, the OMNIC username and the date-time is recorded in the Collection whenever data is collected or modified.

History: This issue occurred in OMNIC version 6.0a. Tracking number: ENH03110.

# If a digitally signed spectrum is modified but not saved, the display of that spectrum would change to "Spectrum not signed". This is not correct as the file saved on disk still has a valid signature.

**Improvement:** Now OMNIC automatically detects when spectrum in memory does not match file on disk and updates the display of the digital signature as needed for in all OMNIC windows. The message "Unable to verify digital signature. The data has been changed" will be displayed when a saved spectrum with a digital signature is modified in OMNIC.

**History:** This issue occurred in OMNIC 6.0a. Tracking numbers: V&V03567 & CST03607.

#### Record the signing of a spectral file in the Collection and Processing Information.

**Improvement:** When a spectral file is signed, the username, date-time, and the reason for the signature are recorded in the Data Processing History section of the Collection and Processing Information.

History: This issue occurred in OMNIC 6.0a. Tracking number: CST02891.

# Added ability to have an NTFS folder with RWX permission (no delete) and allow spectral file saves.

**Improvement:** In previous versions, users need RWX and delete permission to save files to a NTFS folder. FDA requirements for electronic records require additional controls on which user's can delete files. A change was made in OMNIC to allow file saving in a NTFS folder without requiring users to have delete privileges.

History: This issue occurred in OMNIC 6.0a. Tracking number: CST03359.

# Changed atmospheric suppression feature so that during data collection, the suppression is only performed if the result is improved when compared to the result from the unsuppressed spectra.

**Improvement:** If automatic atmospheric suppression is enabled on the Collect Tab in Experiment Setup, the software removes water and carbon dioxide bands from the background and sample single beam spectra. When the Absorbance spectrum is calculated, OMNIC will perform the processing with and without the suppression applied to the single beams. The displayed result will be the resultant Absorbance spectrum with the best baseline characteristics.

**History:** This issue occurred in OMNIC version 6.0a. Tracking number: ENH03215.

### Enhanced axis routines to improve annotation capabilities when spectra are displayed in wavelength.

**Improvement:** Peaks labels were not being displayed correctly when spectra in wavelength were annotated. Note that if a spectrum in wavelength is annotated (for example, peak location) and then the spectrum is converted to wavenumbers, the text for the annotation does not change. Annotations are static text strings.

History: This issue occurred in all prior OMNIC versions. Tracking number: V&V03344.

### Add in capability to call DDE annotate command with only 2 arguments, if no text is specified use the x or x&y position for the annotation text.

**Improvement:** Simplifies the entering if annotations for the most common use of the DDE annotate command.

History: This issue occurred in OMNIC 6.0a. Tracking number: ENH03354.

### Add capability to display information from Almega data files such as laser wavelength and grating in the Collection and Processing Information when viewed in workstation OMNIC.

**Improvement:** Previously, if the Collection and Processing Information of a Raman spectra acquired with an Almega spectrometer was viewed in workstation OMNIC, the Almega spectrometer information was incomplete. OMNIC has been enhanced to show the Almega spectrometer information in the Collection and Processing Information.

**History:** This issue occurred in OMNIC versions 5.2 through OMNIC version 6.0a. Tracking number: V&V02692.

## Changed resource text "The spectra have different Y-axis units." to "The spectra have different axis units." This text was used to refer to different X and different Y-axis units.

**Improvement:** The error message a user would see if for example, they tried to add two spectra of different x-axis units, is now clearer.

History: This issue occurred in OMNIC 6.0a. Tracking number: V&V03356.

#### Added cue card help for various tool palettes within OMNIC.

**Improvement:** Right-clicking on the tool palettes icons will bring up context sensitive help for that icon.

**History:** This issue occurred in OMNIC versions 4.0 through OMNIC version 6.0a. Tracking number: ENH03360.

## Improved COM interface to DDE commands to insert '[' characters if needed and to properly wait for command completion before returning from the command for asynchronous commands.

**Improvement:** Enhanced OMNIC's COM interface to perform it's own checking for proper command syntax and to wait until a previous command has completed before issuing the next DDE command.

History: This issue occurred in OMNIC 6.0a. Tracking number: N/A.

#### Added support to add COM objects to OMNIC functionality at run time.

**Improvement:** Enhanced the functionality of OMNIC's COM interface.

History: This issue occurred in OMNIC version 6.0a. Tracking number: ENH03355.

#### **Resolved Issues**

#### OMNIC

### Request to store the name and path of the background file in the Collection and Processing Information.

**Description:** If the background file comes from the disk, the name and path for the file is captured in the Collection and Processing Information.

History: This issue occurred in OMNIC version 6.0a. Tracking number: ENH02565.

### In the Collection and Processing Information, the data collection error information is displayed on screen but not printed.

**Description:** OMNIC enhanced to print out all information in the Collection and Processing Information.

History: This issue occurred in OMNIC version 6.0a. Tracking number: CST03442.

### If a spectrum was extracted from a notebook, the collection time that appeared in the Collection and Processing Information was that of the last spectra from the lab notebook.

**Description:** The collection time that appears in the Collection and Processing Information is now that of the extracted spectrum.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02646.

# Changed text from "Signature could not be verified" to "Signature could not be verified because the necessary software or operating system is not present." This occurs on Win98 or when DS not purchased.

**Description:** A user can open a digitally signed file on an operating system that does not support the encryption tools. Without these tools, OMNIC knows a signature is there but cannot decrypt the signature.

History: This issue occurred in OMNIC version 6.0a. Tracking number: N/A.

### OMNIC sign read-only files. Put in test for read-only files before attempting to sign them. Now puts up an error message when they are read-only

**Description:** If a file is read-only, an error message will be displayed to the user indicating that the reason the file cannot be signed is that it is read-only.

History: This issue occurred in OMNIC version 6.0a. Tracking number: N/A.

### Performing a search of a digitally signed spectrum changed the status in the display of that spectrum to "Spectrum not signed."

**Description:** Change made to not change the status of the signature due to a search. Searching does not modify the data.

**History:** This issue occurred in OMNIC version 6.0a. Tracking number: CST03526 & V&V03610.

#### Unable to configure a custom detector on the right hand side of the spectrometer.

**Description:** Change made in Bench Configuration application to correctly configure right-hand custom detectors.

**History:** This issue occurred in OMNIC version 6.0a. Tracking number: CST02644 & CST02645.

#### Spectral range for XT-KBr beamsplitter and DTGS TE cooled is not correct.

**Description:** With OMNIC 6.0a, the default range for all sources was 4000 - 400 cm-1. A new default range of 11,000 - 375 cm-1 has been set for the XT-KBr beamsplitter and DTGS TE cooled systems.

History: This issue occurred in all prior OMNIC versions. Tracking number: V&V03368.

#### Changed to allow reset bench at start of Raman data collection.

**Description:** On the Advanced tab of Experiment Setup, the option to "reset bench at start of collection" has been enabled for Raman data collections.

**History:** This issue occurred in all previous OMNIC versions. Tracking number: V&V03112.

#### The sample compartment validation wheel for the Avatar does not work with OMNIC 6.

**Description:** The Avatar driver has been modified to control a sample compartment validation wheel.

History: This issue occurred in OMNIC version 6.0a Tracking number: V&V02860.

### If a Mattson spectrometer had a communication failure when in Experiment Setup, the user had to close and then re-open the Experiment Setup dialog to resume communications.

**Description:** Change to OMNIC so that if a communication failure occurs while the user has the Experiment Setup dialog open, the user can restart communications without exiting Experiment Setup or changing tabs.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03362.

#### Changed OMNIC to not require a default.cfg file on startup. It creates one if needed now.

**Description:** Default.cfg is installed during the OMNIC installation. If the file is not found on startup, OMNIC will now create the file.

**History:** This issue occurred in all prior OMNIC versions. Tracking number: V&V02877 & ENH03369.

### Fixed tiny memory leak when a new background is collected. Only a problem for repeated background collects over days.

**Description:** Small sections of memory were not being freed after a background collection. Over time, this can affect system performance as less memory is available. This has been fixed.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03370.

### Modify Reprocess to account for the fact that an atmospheric suppression might be done on a spectrum with SSP equal to one

**Description:** Reprocess will now account for atmospheric suppression if the Sample Spacing Parameter is set to one.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03373.

#### The Save Group command does not let the user save to a network folder with an UNC path.

**Description:** OMNIC changed to allow UNC paths as the destination folder when saving groups.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03393.

#### OMNIC .SPA files are not associated with the OMNIC application.

**Description:** OMNIC .SPA files will be associated to OMNIC if there is no other association for .SPA files in the registry.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03377.

#### OMNIC could not read in some older PC-IR data files.

**Description:** Fixed a crash that occurred on some systems when OMNIC tried to read in .SPA files created with PC-IR DOS Software.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03371.

### If you save a spectrum as a CSV file, the entire spectrum is being saved to the file instead of only the displayed region.

Description: OMNIC changed so that only the displayed region is saved to the CSV file.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02612.

#### Mattson files other than .abs are not saved properly.

**Description:** Prompting for before overwriting a Mattson file is only done for .ABS files. No prompting if a .RAS, .IFG, or .DRT file is being saved.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02355.

Modified JCAMP-DX to always write out LONGDATE for Y2K compliancy. Additionally, a small change to continue writing out JCAMP-DX the old way for dates less than 2000. That is 10/04/97 and write out dates new 4 digit way when greater than 1999.

**Description:** Long dates were added into the 5.01 JCAMP specification. This has been implemented in OMNIC to assist users with Y2K issues.

**History:** This issue occurred in OMNIC versions 4 through 6.0a. Tracking number: V&V02730.

### If the spectra were being displayed in wavelength, the only option allowed in for an X-axis format in the Display Options was Normal.

**Description:** OMNIC has been changed to allow any of the wavenumber displays when the current x-axis format is in wavelength.

**History:** This issue occurred in OMNIC versions 4 through 6.0a. Tracking number: V&V02240.

#### If the Sampling Information, enabled through the Display Setup dialog in the View menu, did not fit one a single line, the text would not print. Need to correctly determine width of printable area for text wrapping. Fixed issues where if text enabled through Display Options wraps, it would not print.

**Description:** Changes made to correctly determine the width of the printable area. Printing, wrapping text if necessary, fixed for the Sampling Information.

**History:** This issue occurred in OMNIC version 6.0a. Tracking number: V&V02759 & V&V03395.

### Under Display Setup, choosing overlaid titles and displaying sampling information caused the text to overlap.

**Description:** Issue has been resolved by moving the sampling information below the overlaid titles.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03559.

Under Display Setup, choosing overlaid titles and displaying multiple spectra with the Digital Signature option installed caused the titles to overlap the signature information on the display.

**Description:** Issue has been resolved by moving the digital signature information below the overlaid titles.

History: This issue occurred in OMNIC version 6.0a. Tracking number: CST02891.

### The spectral title will not print if an annotation's starting point was near 2500 cm-1. Also, long spectral titles will not print if the title cannot fit on a single line.

**Description:** OMNIC modified to display the spectral title independent of the placement of other annotations. Also, corrected error in printing routine to correctly wrap titles that are longer than a single line.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02759.

### If one copies and pastes an OMNIC window into a program such as MS Word or PowerPoint, it is copied with the New Window axis limits instead of the displayed values.

**Description:** Change to OMNIC so that if an OMNIC window is copied and then pasted into another application, it appears with the current display limits of the OMNIC window, not the values from the Edit/Options/New Window dialog.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03334.

### The Getting Started tutorial would intermittently stop running at the 24<sup>th</sup> screen on Windows 2000 systems.

**Description:** There is a documented problem with ToolBook<sup>®</sup> II applications and Windows 2000. The issue is supposed to be addressed with Windows 2000 SP3. A workaround has been implemented in OMNIC to eliminate the error.

**History:** This issue occurred in OMNIC versions 5 through 6.0a. Tracking number: V&V03497.

#### Enabled cue-card help for Copy and Sign buttons in the report feature.

**Description:** Context sensitive help for the Copy and Sign buttons in View Notebook has been added. The help can be accessed by right clicking on the buttons.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03363

### If the Roll & Zoom command is chosen, pressing F1 for help brings up the help topic for saving configurations.

**Description:** If Roll & Zoom is highlighted in the View menu, the Roll & Zoom help will appear if the user presses the F1 key.

**History:** This issue occurred in OMNIC versions 4 through 6.0a. Tracking number: V&V02510.

#### Added new cue-card ID# definitions for spectrum information dialog

**Description:** Context sensitive help was added to the Collection and Processing Information. The help is accessed by right clicking on the background area of the dialog.

**History:** This issue occurred in OMNIC versions 4 through 6.0a. Tracking number: V&V02512.

#### Help menu items are not be displayed according to the Edit Menu configuration.

**Description:** A change was made in Edit Menu to not let the user disable or hide menu items that are submenu headings such as "Learning OMNIC" and "Sampling Techniques". Other

items in the help menu can now be disabled or hidden as determined by the configuration constructed with Edit Menu.

**History:** This issue occurred in OMNIC versions 4 through 6.0a. Tracking number: CST03574.

### If "Text Only" is selected for the OMNIC Toolbar, the toolbar button separator and the button frame do not appear.

**Description:** Changed OMNIC to show the separators and the button frames if "Text Only" is selected as the toolbar type.

**History:** This issue occurred in OMNIC version 6.0a. Tracking number: V&V02497 & V&V02714.

### The Command Text label in the Add Item Dialog in Edit Menu is not changing consistently with the Item Type.

**Description:** Depending upon the Item Type, the title for the Command Text box changes. Scenarios existed where the text string did not match the Item type. This has been fixed.

History: This issue occurred in OMNIC versions 4 through 6.0a. Tracking number: V&V02535

### The colon after "Experiment" for the experiment drop down control on the main OMNIC window is hidden.

**Description:** The Text string was repositioned on the main OMNIC to show the colon.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02537.

### Fixed issue when if the computer's display mode was set to 256 or less colors, the subtract auto Y check box could not be checked.

**Description:** In the Subtract window, the auto Y check box can be selected for all video display modes on the computer.

**History:** This issue occurred in OMNIC version 6.0a. Tracking number: V&V02673.

#### Update look of "Change data spacing" dialog to match new OMNIC 6 blue textured look.

**Description:** OMNIC 6 enabled the user to choose the OMNIC Window Style in the Edit/Options/View dialog. The style was not applied to the Change Data Spacing dialog in the previous OMNIC version.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03367.

#### **Basic Macros and Macros Pro**

#### Some Basic Macros would crash intermittently when run from the OMNIC toolbar.

Description: Change made to Macros Basic.

History: This issue occurred in Macros Basic version 6.0. Tracking number: V&V02674.

### Modified variance command to put result(s) in current window instead of a new window if the command is not invoked from DDE.

**Description:** Change was made in OMNIC so that Variance command functioned the same as it had with OMNIC 5.0. By invoking the command: ExecuteOMNIC "Variance 1", the average is calculated and added to current window.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03320.

### Modified "Statistical Spectra" to not show New Window prompt if command invoked from DDE

**Description:** Change was made in OMNIC so that Statistical Spectra functioned the same as it had with OMNIC 5.0. By invoking Statistical Spectra though DDE, the result will be added to the current OMNIC window.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03320.

#### InterpretIR+

### InterpretIR+ does not automatically import the active spectrum from OMNIC when launched.

**Description:** InterpretIR+ has been changed to automatically import the active spectra when InterpretIR+ is launched from the OMNIC Analyze menu.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02713.

#### Atlµs, µView<sup>™</sup> (Microview) and View Stage

#### Expanded support to allow Atlµs maps to contain up to 50,000 spectra.

**Improvement:** Previous versions of Atlµs allowed users to collect just less than 16K spectra in a map. The limit has been increased to 50,000.

History: This issue occurred in Atlµs v2.5. Tracking number: ENH03351.

### Request to save the image size when Atlµs (or Microview) is closed so that the program automatically recalls the values for the user.

**Description:** The last used video size is now saved when Atlµs (or Microview) is closed. The saved value is loaded and used when Atlµs (or Microview) is started.

History: This issue occurred in Atlµs version 2.5. Tracking number: V&V00958.

### Request to set the number of background and sample scans to different values in Map Setup within Atlµs.

**Description:** The user can specify a different number of scans for a background versus a sample scan in Atlµs.

History: This issue occurred in Atlµs version 2.5. Tracking number: V&V00637.

#### Atlus does not autofocus for each video frame when collecting a mosaic with a map

**Description:** Changed Atlµs so that if "autofocus at each point" is selected/enabled, the Mosaic will also autofocus at each point.

History: This issue occurred in Atlµs version 2.5. Tracking number: V&V02693.

#### Microview opens in a small window after installation.

**Description:** The size of the Microview application has been increased to allow the user to more easily view the controls.

History: This issue occurred in Microview version 2.5. Tracking number: V&V02771.

#### The ruler in the navigation pane of Atlµs cannot be moved with the mouse.

**Description:** Change made so that the if a ruler is drawn in the navigation pane, the arrow tool can be used to position the ruler.

History: This issue occurred in Atlµs version 2.5. Tracking number: V&V03313.

### Clicking on focus control in Atlµs or Microview causes the stage focus to run-on unexpectedly

**Description:** The stepping increment for the Z-axis control was changed to a finer granularity. The stage moves one increment with each mouse click.

History: This issue occurred in Atlµs version 2.5. Tracking number: V&V02772.

### With the View Stage, the Experiment Setup interferogram display freezes after toggling the lamp on and then off.

**Description:** View Stage controls in Experiment Setup can now be toggled/changed without freezing the interferogram display.

**History:** This issue occurred in OMNIC version 6.0a. Tracking number: V&V02774 & V&V03374.

### View Stage users cannot access Atlµs or $\mu$ View (Microview) correctly. Provide a calibration file for the View Stage so that users can then use Atlµs or $\mu$ View.

**Description:** A View Stage calibration file is needed. The file "ramanvs.cal" has been included in the factory folder.

History: This issue occurred in Atlµs version 2.5. Tracking number: V&V02770.

#### Val-Q

#### Spectral group collected in Val-Q could not be saved to a network drive.

**Description:** User now has the choice as to where the spectral data is saved. Can be to any mapped local or network drive.

**History:** Problem occurs in <Product Name> version <Number>. Added to release notes in <Month> <Year>. Tracking number: CST02895.

### OMNIC experiment parameters are not being restored to previous settings when Val-Q closes.

**Description:** Val-Q modified to store current OMNIC settings when Val-Q starts and restore them when Val-Q closes.

**History:** Problem occurs in <Product Name> version <Number>. Added to release notes in <Month> <Year>. Tracking number: CST03178.

#### Series

#### Fixed bug that prevented import of TGA files into series.

**Description:** A change occurred in OMNIC version 6.0a that prevented TGA files from being imported into OMNIC. This has been fixed.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02633.

### Series and Atlµs progress bar now painted with new OMNIC 6 blue textured dialog style colors

**Description:** OMNIC 6 enabled the user to choose the OMNIC Window Style in the Edit/Options/View dialog. The style was not applied to the Series or Atlµs progress bars in the previous OMNIC version.

**History:** This issue occurred in OMNIC version 6.0a and Atlµs version 2.5. Tracking number: V&V03364.

#### Fixed series setup dialog to only allow values to be entered that create valid series files. Prevents attempt to create multi-gigabyte files that caused the display of the size to be a

negative number or when the number of spectra exceeded 60000. Modified routine that calculates Atlµs map file size to return 0 if resultant file would be larger than is supported. Also file creation to return 0 if too many spectra in potential file (more than supported).

**Description:** Some combinations of series collect parameters would cause the Estimated File size in the Series Setup dialog to display a negative number as it overflowed the variable. Limits and error checking have been added to ensure that a valid estimated file size is displayed.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02699.

#### When profiling Series or Atlµs data, ignore the data spacing test for a measure only method

**Description:** The data spacing is not checked when a measure only method is applied to Series or Atlµs data.

History: This issue occurred in OMNIC version 6.0a. Tracking number: CST03372.

#### Series collect window does not always update if very data is acquired rapidly.

**Description:** Enhance Series collect so that the current spectrum always updates the display even when the time increment is less than one expected increment.

History: This issue occurred in OMNIC version 6.0a. Tracking number: ENH03376.

### Using split bi-directional rapid scan often resulted in dropped scans when going faster than about 60 scans per second

**Description:** The time stamp increment for rapid scan was changed to a finer resolution so that all scans would have a unique time stamp.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02344.

### If one uses the same peak and baseline values for the numerator and denominator in Profile setup for "Peak height ratio of two peaks", the Y readout was displayed as "1.#QQ".

**Description:** Readout now displays the correct value.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V03322.

#### Almega

### Added Photobleach time to collect tab; removed estimated resolution as it is on the Bench tab.

Description: New Feature.

History: Feature added to OMNIC for Almega v6.1.

### Added partial wavelength calibration feature. This lets the user select a subset of spectral ranges to calibrate if they don't want to take the time to calibrate all ranges.

Description: New Feature.

**History:** Feature added to OMNIC for Almega v6.1.

Changed the alignment procedure to start at the center and spiral out rather than raster a rectangle.

**Description:** New Feature.

**History:** Feature added to OMNIC for Almega v6.1.

#### Coarse adjustment needs a finer scale.

**Description:** Coarse adjustment increment reduced. Allows for smoother operation and less overshoot.

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: V&V03598

### If the focus button is clicked rapidly with a 50x objective, the focus motors may not be able to bring the object back in focus. Manual refocusing required.

**Description:** Coarse adjustment increment reduced. Allows for smoother operation and less overshoot.

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: V&V03601

### The signal is not changing during autoalign if option 3, align laser to pinhole, is selected. **Description:** <Insert Description Here>.

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: V&V03570.

#### Wavelength calibration. Improved algorithms to make calibration more robust.

**Description:** Added code to adjust spectrograph focal length for best fit. Added neon lines (neonhigh.txt and neonlow.txt files) to do a better job covering the spectral range for each grating position. Removed some chronically mismatched neon lines. Results are saved in a single file, calibrate.txt, rather than individual peak####.txt files.

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

#### Laser calibration improvements.

**Description:** Changed peak location algorithm to use center-of-gravity. Modified procedure so that second laser is calibrated even if first laser fails. Fixed bug that caused some single laser configurations to hang up. Fixed bug so that a combined bin range is calculated for single laser systems.

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

#### Almega Installation Issues.

**Description:** Removed code which caused default.con and default.exp files to be write protected. Fixed issue which installed the WinNT 4.0 driver under Windows 2000 in addition to the Windows 2000 driver.

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

#### Do laser accordian before Set\_fold\_limits to get desired range.

#### **Description:**

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

#### Require a laser normalize for atypical laser type spectrometers.

#### **Description:**

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

#### Add methods to calculate the resolution information for atypical lasers.

#### **Description:**

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

### Changed startup code to detect when bench power is off and prevent showing multiple camera errors.

#### **Description:**

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

Added initialization code so that the correct grating is selected when entering the Bench or Align tab. This also fixes bug, which caused occasional blank spectral range text boxes when selecting 532 Low Res grating.

#### **Description:**

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

### Automatic data spacing option on Advanced tab not always selected by default. Changed so it is initialized to checked.

#### **Description:**

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

### Turn both lasers On/Off option on Advanced tab does not stay selected. Disable this option if only one laser installed.

#### **Description:**

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A./A.

#### Fixed bug that occasionally introduced a blank data point in spliced spectra.

#### Description:

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

#### Added code to bin-in-memory collects to check for CCD traps.

#### **Description:**

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

### Modified DDE commands so that calibrations can be run from macro (no finish dialog) and un-invoked collects finish correctly.

#### Description:

History: Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

### Spectrograph alignment tab changed so that if LED is at high intensity during pinhole align, Max contains "(H)", if at low intensity it contains "(L)".

#### **Description:**

**History:** Issue occurred in OMNIC for Almega v6.0a. Tracking number: N/A.

#### SST and TRS

#### Added multiple scan capability to all of the Step Scan menus.

#### **Description:** New Feature.

History: This feature was added in OMNIC version 6.1. Tracking number: N/A.

#### Added multiple trigger for Time Resolved Step Scan (TRS).

Description: New Feature.

History: This feature was added in OMNIC version 6.1. Tracking number: N/A.

#### Provide TRS drivers for Gage acquisition boards on the Thermo Nicolet installation CD Description: New Feature.

History: This feature was added in OMNIC version 6.1. Tracking number: N/A.

#### Reduced the minimum trigger interval required for TRS experiments.

Description: New Feature.

History: This feature was added in OMNIC version 6.1. Tracking number: N/A.

### Advanced diagnostic test parameters for TRS for the Gage 8500 board were not optimal. The number of samples is being set to zero.

**Description:** The 8500 board is a faster board. Parameters have been updated.

History: This issue occurred in OMNIC version 6.0a. Tracking number: V&V02542.

#### **Known Issues**

### IR Spectral Interpretation will not display the functional group information (accessed by clicking on the eyeglasses) if Library Manager is open.

**Description:** IR Spectral Interpretation will not display the functional group information (accessed by clicking on the eyeglasses) if Library Manager is open

**Recommendation:** The Library Manager window must be closed to view the functional group information and structures.

History: Problem occurs in OMNIC 6.1

#### **OMNIC Installation Directories**

When you install OMNIC the default (recommended) directories depend on whether an earlier version of OMNIC is on your system.

If an earlier version is not present, the default folders are C:\My Documents\OMNIC for data files, and C:\Program Files\OMNIC for program (executable) files and Help files. Within the C:\My Documents\OMNIC folder, the following folders will be created: Autosave for saving spectra automatically after a data collection, Icons for icon image files you can use when customizing the OMNIIC toolbar, Libs for spectral library files, Log for the OMNIC log (if enabled), Macros for OMNIC macro files, Quant for quantitative analysis methods, Param for experiment files and configuration files, Report for report notebooks, and Spectra for spectral data files. Other optional software programs may add other folders to the C:\My Documents\OMNIC folder.

If an earlier version of OMNIC is present, the default data directory is the directory where the earlier version was installed (usually C:\OMNIC). The default directory for program files is where the earlier version was installed (usually C:\Program Files\OMNIC).

In either case, you can specify that other directories be used if desired.

In addition to these directories, OMNIC installs the runtime ToolBook<sup>®</sup> 5.0 files in the Windows\Asym\Runtime directory and the runtime ToolBook 6.0 files in the Program Files\ Asymetrix\Shared Tools\tbsystem directory. These files are used by OMNIC Macros\Basic<sup>TM</sup> and the tutorials.

#### Problems?

For Technical Support, please contact: Thermo Fisher Scientific 5225 Verona Road Madison WI 53711-4495 U.S.A. Telephone: 1 800 532 4752 E-mail: us.techsupport.analyze@thermofisher.com World Wide Web: http://www.thermo.com/spectroscopy

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