

NICDOM Kidney Stone Analysis Kit User's Guide



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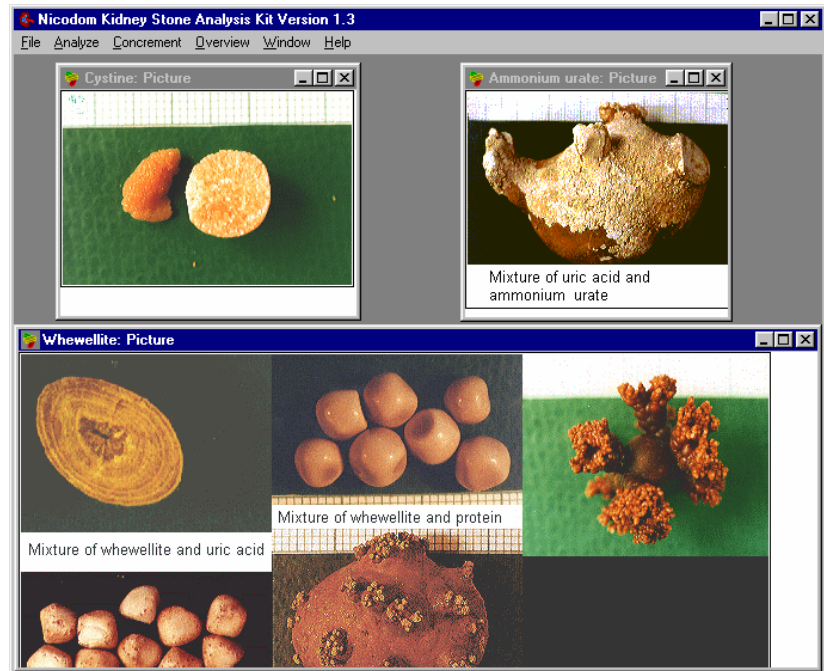
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Introduction

The NICODOM Kidney Stone Analysis Kit was created by spectroscopists and medical doctors to allow analysis of kidney stones using Thermo Electron FT-IR spectrometers running Thermo Electron's OMNIC™ spectroscopy software. This software package has three components:

- Kidney Stone Library Basic
- Kidney Stone Analysis Software
- Kidney Stone Software Guide



Kidney Stone Library Basic

The Kidney Stone Library Basic contains 756 FT-IR spectra of synthetic kidney stone samples. The synthetic samples were prepared by mixing various combinations of pure standard materials. A complete listing of the compounds in the Kidney Stone Library Basic is provided in this manual.

Use the OMNIC Search functions to search the spectrum of an unknown kidney stone against the library spectra. Samples in which the major components are in the concentration range between 30 and 70% produce the best search results (error less than 5%). Real urinary concrement contains a small amount of unknown matrix. This matrix consists mainly of organic components which produce strong absorption bands around 3000 cm^{-1} . For this reason, we recommend using the region from $2000\text{-}450\text{ cm}^{-1}$ for the library search.

Kidney Stone Analysis

Use the Analyze Mode of the Kidney Stone Analysis software to perform a combination of qualitative and quantitative analyses on an unknown kidney stone sample. The software uses a special algorithm to search the spectrum of an unknown sample against a coded library of over 18,000 spectra. The match values from the search results are used to calculate the concentrations of the components in the unknown sample. The results include a reliability factor for the analysis, which can be stored with the sample spectrum. The software provides features that allow you to easily display the spectrum of the unknown sample along with the library reference spectrum so that you can compare their spectral features.

The coded library includes spectra of common artifacts and rare stones. If the analysis software determines that the unknown sample spectrum is distorted or does not come from a kidney stone sample, the software will stop the analysis.

This software package includes 212 spectral data files obtained from real kidney stones (found in human kidneys) and 23 spectral files of major pure components to demonstrate the capabilities of the NICODOM Kidney Stone Analysis Kit. A listing of the file names of the example spectra is provided in Appendix B.

Kidney Stone Software Guide

Use the Kidney Stone Software Guide to search for additional information about the components in a kidney stone sample. This Guide includes interpreted infrared spectra of kidney stone samples and pure chemicals, as well as pictures of stones, explanations of why and how they form, plus structural formulas and optical properties of kidney stones, Raman spectra, a table of spectral peaks, and descriptions of other methods of chemical analysis (qualitative, semi-quantitative, quantitative). In cases where the reliability factor of the IR analysis is low, this guide outlines further steps to verify the composition of the unknown samples. The Guide also provides a brief overview of the medical aspects of kidney stone analysis, such as diagnosis and therapy.

System requirements

Kidney Stone Library and Analysis Software operates on computers equipped with at least the following minimum requirements:

Microsoft® Windows® 98, Windows 2000, or Windows XP.
We recommend the latest service pack.

OMNIC, version 6.0 or higher.

A video card and corresponding Windows driver
that supports 65,000 or more colors

Note If your computer does not have this type of video card, the software will run correctly, but the pictures will not be displayed using the proper colors. ▲

Installing the software

To install the NICODOM Kidney Stone Analysis Kit:

- 1. Start Windows.**
- 2. Insert the Kidney Stone software CD (your CD drive is supposed to be D:/ in following text)**
- 3. Click on the Start button and then click Run.**
- 4. Type or browse to D:/Install_Kidstone_1.3.exe and then press Enter.**

Follow the instructions that appear on the screen. The software serial number is a part of your documentation. A program group and program icon will be created automatically.

- 5. Type or browse to D:/Install_Kidstone_Basic.exe and then press Enter.**

Follow the instructions that appear on the screen. The software serial number is a part of your documentation.

6. Choose International from the Windows control panel and set the following parameters:

Set the decimal separator to a point.

Set the list separator to a comma..

If you choose any other setting, the Kidney Stone Library and Analysis Software may not function properly.

Installation file details

The file "Install_Kidstone_1.3.exe" is an installer of the NICODOM Kidney Stone Analysis Kit Version 1.3. The installer will install following files to the chosen directory. We recommend to use the default installation directory <C:/Kidstone>

Kidney Stone 1.3.exe — This is an executable program file of the NICODOM Kidney Stone Analysis Kit Version 1.3.

stonecod.lbd and stonecod.lbt — These are the files of the coded library needed for the "Analyze OMNIC active" function.

Once you run the executable file, this will automatically set up the library directory path in OMNIC. This setting is invisible. The "Analyze OMNIC active" function of your Kidney Stone software will not work properly if the coded library files are not present in the same directory as the "Kidney Stone 1.3.exe" file.

00.spa - 24.spa — Spectral files needed for the Visual Comparison function. Read only files. Do not delete, rename, or process these spectra. The Visual Comparison function of your Kidney Stone software will not work properly if the original spectra are not present in the same directory as Kidney Stone 1.3.exe.

Kidstone_Spectra_Examples directory — The Kidstone_Spectra_Examples directory contains 212 example spectra. Those spectra allow you to test the software in case you do not have any example spectra available. The spectra can be present in any directory.

Install_Kidstone_Basic.exe — The file Install_Kidstone_Basic.exe is an installer for NICODOM Kidney Stone Library Basic. This program installs the files kidstone.lbd and kidstone.lbt into a directory of your choice. We recommend that you use the default installation directory. Refer to the documentation that came with your OMNIC software for more information about setting a library directory path.

Note If the installation fails from any reason, all mentioned files are on the CD in the directory "Kidstone files". You can install them manually. You can also run the programs from this directory without installation. ▲



Using the Software

Using Kidney Stone Library Basic

The Kidney Stone Library Basic is a standard spectral library, designed to be used with Thermo Electron's OMNIC spectroscopy software. The library runs independently from the NICODOM Kidney Stone Library Kit.

The on-line Help system and other documentation that came with OMNIC contain complete instructions for using spectral libraries. Check the index for the Search command for more information.

Starting the analysis software

There are three ways to start the NICODOM Kidney Stone Library Kit after it has been installed:

- by clicking the icon at the desktop
- by choosing Kidneystone 1.3 from Start/Programs
- by clicking Kidney Stone 1.3.exe in the installation directory

You can also run the program without installing it. Simply insert the CD into your computer, browse to the /Kidstone files/ directory and then click Kidney Stone 1.3.exe.

Analysis software overview

The Kidney Stone Software Guide is an integrated part of the NICODOM Kidney Stone Analysis Kit. Use the Kidney Stone Software Guide to search for additional information about the primary components in a typical kidney stone sample.

The table that follows describes the commands that allow you to display the various information windows for a given component.

Note If a menu item or an information check box is inactive (grayed), the corresponding information is not available for the selected component. ▲

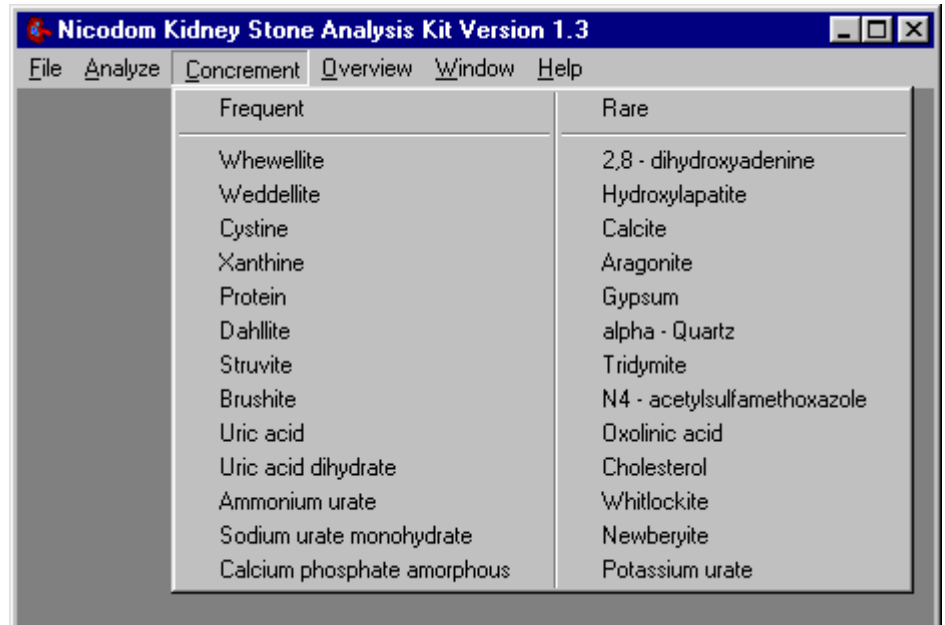
<i>Menu</i>	<i>Command</i>	<i>Description</i>
File	Exit	Use the Exit command to quit the Kidney Stone Library and Analysis Software.
Concrement		Use this menu to display information about a kidney stone component. The Concrement Menu contains a two-column list of components.
	Component name	To display information about a component, click the component name in the menu. The following dialog box will appear showing the categories of information that can be displayed for the component you selected.
	Information category	To display a category of information, turn on the corresponding check box and choose OK. To turn a check box on or off, click in the box. The check box is on when an X appears in the box and off when the box is blank. When you are finished with an information window, click the close box in the upper right corner of the window to close the window.
		<i>continued...</i>

<i>Menu</i>	<i>Command</i>	<i>Description</i>
Overview		Use this menu to display general information about kidney stone analysis. The following information windows are available.
	Physical methods	Provides information about the various methods available for analyzing urinary concrements and summarizes the advantages and disadvantages of each.
	Peak table	Gives an overview of how to interpret the spectral data from substances that are commonly found in urinary concrement samples.
	Diagnosis	Provides information about the medical aspects of kidney stones.
	Therapy	Provides information about the medical aspects of kidney stones.
	Chemical analysis	Describes the qualitative and quantitative methods for analyzing all cations and anions found in urinary concrement samples.
	Reference	Lists a number of books and papers about kidney stones.
	Causes & occurrence	Provides supplementary medical information about the selected component.
	Optical properties	Describes the crystal forms of the selected component.
	Chemical analysis	Gives a brief overview of the quantitative, semi-quantitative and qualitative methods that are typically used to analyze the selected component.
	Chemical formula	Displays the mineralogical name, chemical name, and the chemical and structural formulas for the selected component.
	Picture windows	Use the Picture check box in the component information dialog box to display a photographic image of a real concrement sample that contains the selected component. A description of the sample is also provided.
		<i>continued...</i>

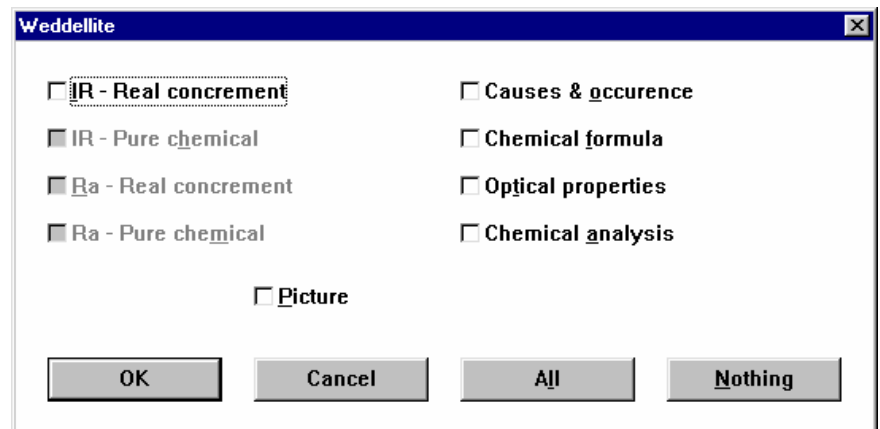
<i>Menu</i>	<i>Command</i>	<i>Description</i>
Overview	All	If you want to display all of the available information for the selected component, click the All button in the dialog box.
	Nothing	To close all of the open information windows at one time, choose the component name from the Concrement menu and then click Nothing.
Window		Use the commands in this menu to select an open window, to arrange windows that have been minimized, or to arrange all of the open windows in a cascade or in tiles across the screen.
Help menu	About	Use the About command in the Help menu to display copyright information about the Kidney Stone Library and Analysis Software.

Concrement menu

As shown below, the Concrement Menu contains a two-column list of components. The components are arranged by the frequency of their occurrence in real kidney stones.

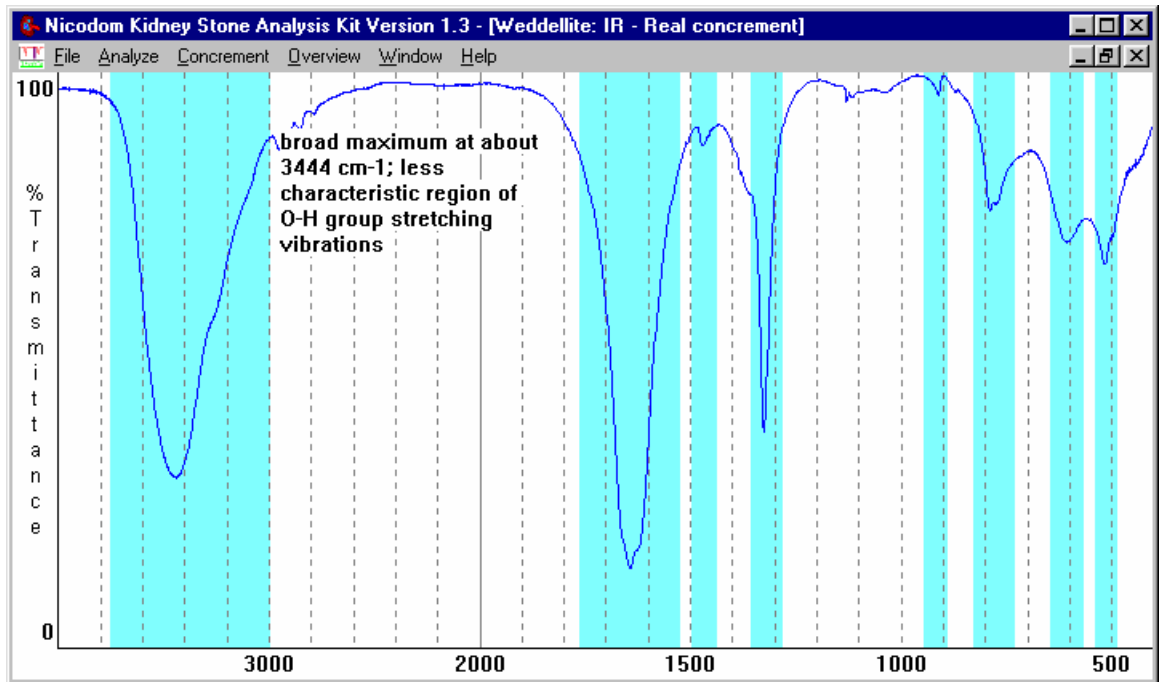


Once you select a particular component, a component dialog box opens and allows you to select particular information you would like to review. The illustration that follows shows a typical component dialog box.

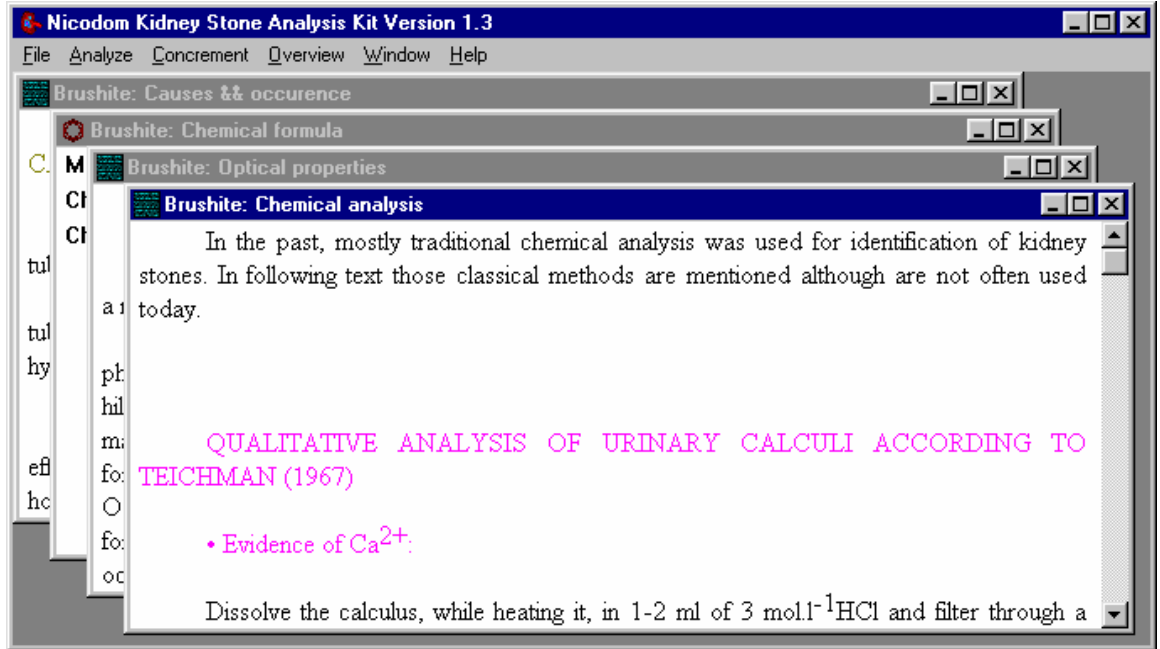


Use the four check boxes on the left side of the component information dialog box to display the infrared or raman spectrum of an actual concrement sample or the pure chemical of the selected component.

The following illustration shows the infrared spectrum of a real concrement sample, calcite. Spectral peaks or regions that are highlighted in blue contain additional information. Click anywhere in a highlighted area to display a description of the spectral peak or region.



Use the four check boxes on the left side of the component information dialog box to display textual information about actual concrement sample or the pure chemical of the selected component. The illustration that follows shows a cascade of the information windows available for concrement sample, Brushite.

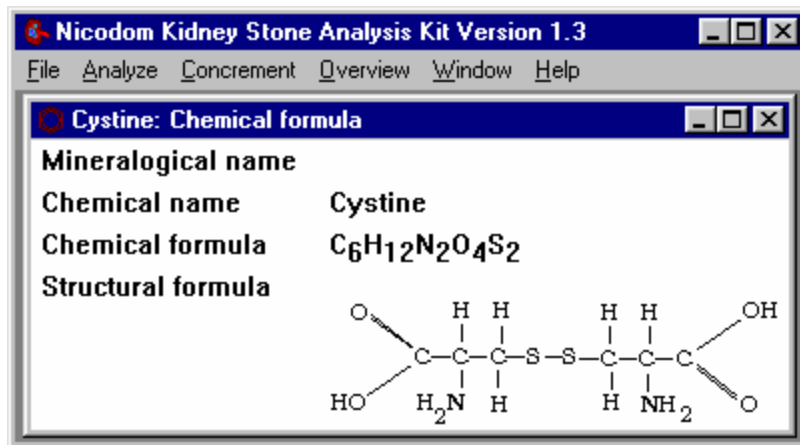


Causes & occurrence — This window provides supplementary medical information about the selected component.

Optical properties — The optical properties window describes the crystal forms of the selected component.

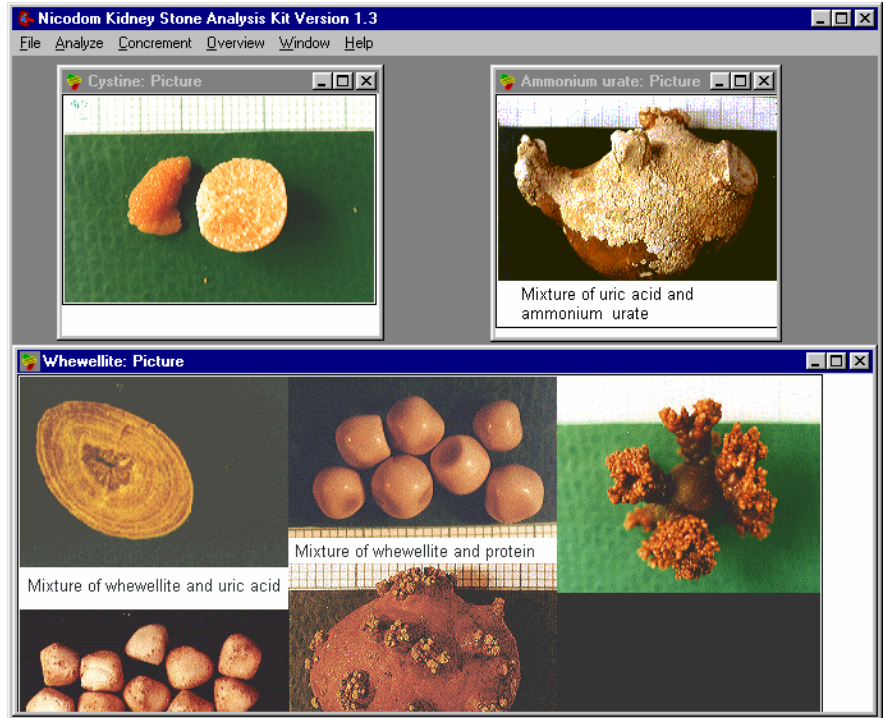
Chemical analysis — The chemical analysis window gives a brief overview of the quantitative, semi-quantitative and qualitative methods that are typically used to analyze the selected component.

Chemical formula — The chemical formula window displays the mineralogical name, chemical name, and the chemical and structural formulas for the selected component. The following illustration shows the chemical formula window for cystine.



Note To expand the chemical formula window to its original size, use the right mouse button and click inside the window. ▲

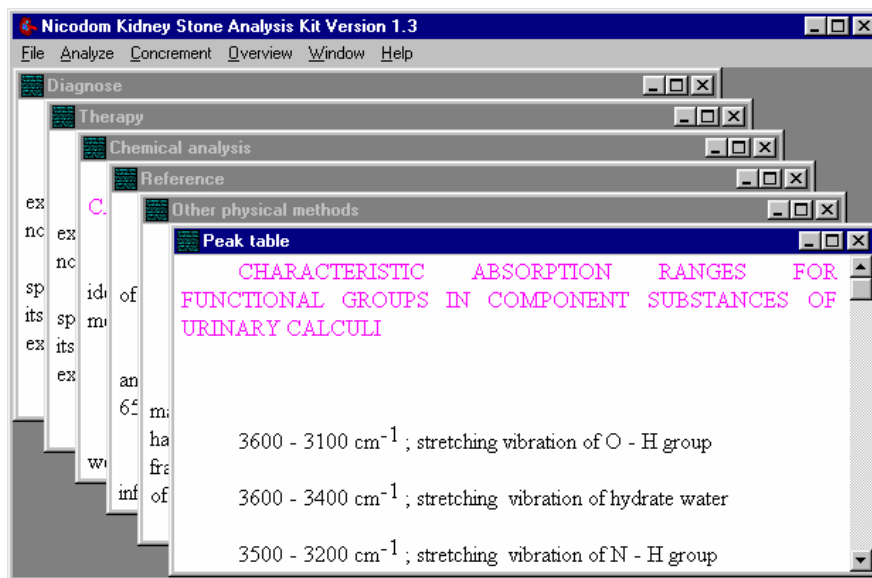
Picture — Use the Picture check box in the component information dialog box to display a photographic image and description of a real concrement sample that contains the selected component.



Note To expand the picture window to its original size, use the right mouse button to click inside the window. ▲

Overview menu

Use this menu to display general information about kidney stone analysis. The illustration that follows shows a cascade of the Overview menu windows.



Physical methods — This window provides information about the various methods available for analyzing urinary concretions and summarizes the advantages and disadvantages of each.

Peak table — Use the peak table window to get overview information about interpreting the spectral data from substances that are commonly found in urinary concrement samples.

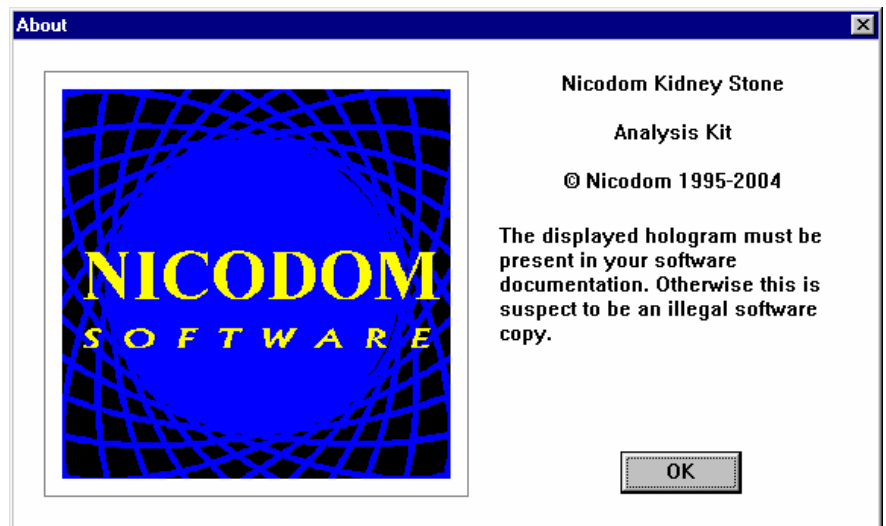
Diagnosis and therapy — The diagnose and therapy windows provide information about the medical aspects of kidney stones.

Chemical analysis — The chemical analysis window describes qualitative and quantitative methods for analyzing all cations and anions found in urinary concrement samples.

Reference — To obtain lists a number of books and papers about kidney stones, open the Reference window.

Window menu Use the commands in this menu to select an open window, to restore windows that have been minimized, or to arrange all of the open windows in a cascade or in tiles across the screen.

Help menu Use the About command in the Help menu to display copyright information for the Kidney Stone Library and Analysis Software.



Exiting the analysis software You should quit the NICODOM Kidney Stone Library Kit before shutting down your computer. To quit the Kidney Stone software choose Exit from the File menu.



Analyzing Samples

This chapter provides more information about using the NICODOM Kidney Stone Kit to analyze samples. The software has been designed and tested with samples collected using the KBr pellet technique. If you use other than KBr pellet technique, this may influence the software performance.

Preparing samples for analysis

To insure accurate analytical results, prepare each kidney stone sample according to these instructions.

Make sure you use representative samples for the analysis.

Since most kidney stones are not homogeneous, we recommend that you analyze four samples of each kidney stone

Take one sample from the core, one from the middle, one from the surface and a sample from the homogenized stone.

Each sample should be mixed with potassium bromide to form a standard KBr pellet used for infrared analysis.

A 13 mm pellet should contain 0.1-0.5 mg of concrement sample and about 200 mg of potassium bromide.

The pellet should be free of moisture (transparent) although some water is often present in the sample.

Important

Do not make the KBr pellets until you are ready to collect the sample data. You must collect the spectrum of each sample immediately after you finish making the pellet. ▲

Analyzing samples

Follow the instructions that follow to analyze the spectrum of a kidney stone sample:

Important

The files "00.spa - 24.spa" are the spectral files required by the Visual Comparison function. Do not delete, rename, process these spectra. The Visual comparison function of your Kidney Stone software will not work properly if the original spectra are not present in the same directory as the "Kidney Stone 1.3.exe" file. ▲

- 1. Open the OMNIC spectroscopy software application.**
- 2. Open and select the spectrum of the sample you wish to analyze.**
- 3. Open and select the Kidney Stone Analysis Kit application.**

Note

You can use the Alt + tab keys to switch between the two applications. ▲

- 4. From the main software screen for the Kidney Stone Library and Analysis Software, choose OMNIC Active from the Analyze menu.**

Wait while the software analyzes the spectrum you selected. In most cases, the analysis takes about 20 seconds. When the analysis finishes, the results are displayed. The illustration that follows shows a typical analysis results window.

Advanced Analysis [X]

Spectrum title **Brushite and Weddellite**

Collected **Nov/06/2001, 17:10:53**

Component	Content
Brushite	70 %
Weddellite	23 %
Matrix (unknown matter, usually protein)	7 %

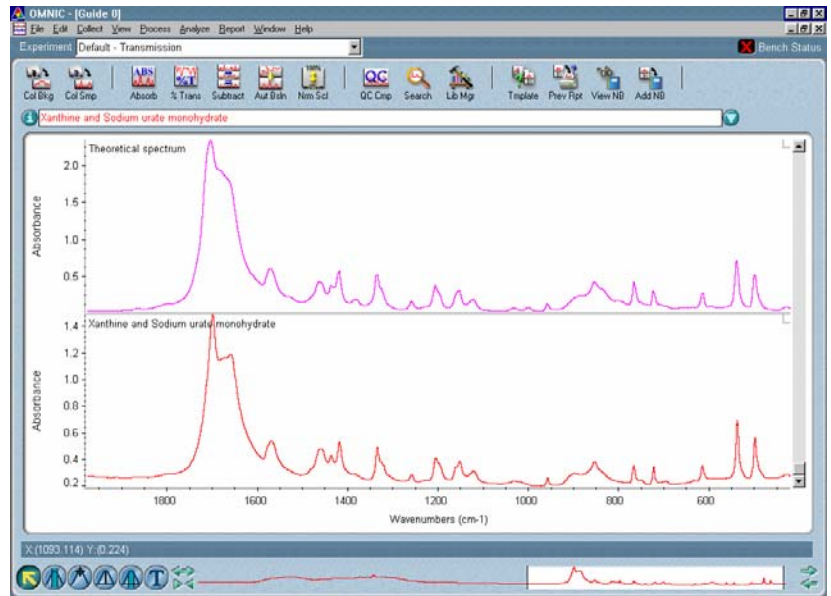
Reliability index 94 - Result is very reliable

The title of the spectrum and the date and time the spectrum was collected are displayed at the top of the window followed by a table of data. The table displays the names and concentrations (in percent) of up to five components. If matrix (organic) material is present in the sample and the material can be identified, a matrix concentration value will also be provided. A summary of the analysis results and a reliability index appear immediately below the table.

5. To see the reference spectrum that was used for the analysis, choose Visual Comparison.

The reference spectrum is obtained by mixing the pure component spectra. The reference spectrum and the unknown sample spectrum appear in an OMNIC spectral window. The two spectra are displayed in stack mode so that you can easily compare their spectral features.

If the theoretical spectrum is different from spectrum of your sample, the analysis result is not reliable. Try the spectral SEARCH using the basic or coded libraries or refer to Kindey Stone Guide for other methods.



Note When you are finished viewing the spectral data, switch back to the Kidney Stone software (press Alt + tab). ▲

- 6. To see the table of reliability data, click the Reliability button in the analysis results window.**

When you are finished reading the data, click OK to return to the analysis results window.

- 7. You can easily store the analysis results in the spectrum comments by clicking the Comment button in the analysis results window.**

The results are stored in the Comments section of the spectrum's Collection and Processing Information dialog box.

Important

Any comments that are currently stored in the Comments box for the selected spectrum will be overwritten. ▲

- 8. When you are finished reviewing the analysis results, choose OK to close the results window.**

Troubleshooting analysis failures

The precision that can be achieved with this type of analysis varies with the type of concretment, the concentrations of the components in the sample, the type and amount of correction applied to the spectral baseline and the amount of impurities that are present in the sample. In addition, any components which are present in the sample but in concentrations that are less than 10% will not be detected. If a component concentration falls between 10 and 15%, a concentration value will be reported but the result will not be very reliable.

Occasionally, an analysis using the Kidney Stone Library and Analysis software will be unsuccessful. In that event, use the information that follows for possible causes and solutions.

<i>Error message</i>	<i>Possible cause</i>	<i>Solution</i>
Analysis failed	OMNIC is not running.	Open OMNIC
	No spectrum selected.	The spectrum you want to analyze must be displayed and selected.
	Too many spectra selected.	No additional spectra can be selected.
	Incorrect spectral range	The spectral range for the selected spectrum must include the range between 400 and 2000 cm ⁻¹ .
	Incorrect threshold limits.	The threshold limit for the OMNIC Search command must be set to zero.
OMNIC Search is still open.	Close the Search window. The OMNIC Search window must be closed when you initiate the OMNIC Active command in the Kidney Stone Analysis Software.	
		<i>continued...</i>

<i>Error message</i>	<i>Possible cause</i>	<i>Solution</i>
The spectrum is distorted.	The region between 400 and 2000 cm^{-1} contains a highly absorbing band. (> 2 absorbance units)	
Rare or drug concrement, other than kidney stone spectrum.	The spectrum of the unknown sample does not match any of the typical kidney stone spectra that are stored in the data base but the spectrum is similar to one of the other spectra in the data base.	
Analysis unsuccessful. Similar spectrum is not in the library.	The spectrum does not match any of the spectra in the data base	
Unusual concrement, other than kidney stone spectrum, distorted spectrum.	An unknown organic compound is present in the sample.	
Matrix (unknown matter, usually protein) = X%	The matrix material and its concentration is less than 20%	This is the main difference between the spectra of real kidney stones and the synthetic kidney stone spectra. The concentration of organic (matrix) material in real kidney stones varies from 5 to 15%, depending on the type of stone.
Matrix content is unusually high. Similar spectrum is not contained in the library.	The concentration of the matrix material is greater than 20%, the sample is either a very rare (drug) concrement or an artifact and the search will probably fail.	
The "Visual comparison" function does not work properly.	he sample contains both uric acid and its dihydrate, the sum of both forms are reported since the spectra of these two compounds are very similar.	The summed result will be listed under the label "uric acid." From a clinical point of view, the hydrate state of uric acid is irrelevant.



Appendix A — Index of Compounds

This section provides a listing of the compounds in the Kidney Stone Basic FT-IR Library. The spectra are listed by library index number with the names of up to three primary components appearing to the right of the number.

1	90% Weddellite 10% Whewellite	45	90% Whewellite 10% Ammonium Hydrogen Urate
2	Ammonium Hydrogen Urate	46	90% Struvite 10% Whewellite
3	Uric Acid	47	80% Struvite 20% Whewellite
4	Brushite	48	70% Struvite 30% Whewellite
5	Weddellite	49	60% Struvite 40% Whewellite
6	Cystine	50	50% Whewellite 50% Struvite
7	80% Weddellite 20% Whewellite	51	60% Whewellite 40% Struvite
8	Whewellite	52	70% Whewellite 30% Struvite
9	Struvite	53	80% Whewellite 20% Struvite
10	Uric Acid Dihydrate	54	90% Whewellite 10% Struvite
11	70% Weddellite 30% Whewellite	55	90% Dahllite 10% Whewellite
12	60% Weddellite 40% Whewellite	56	80% Dahllite 20% Whewellite
13	50% Whewellite 50% Weddellite	57	70% Dahllite 30% Whewellite
14	60% Whewellite 40% Weddellite	58	60% Dahllite 40% Whewellite
15	Dahllite	59	50% Whewellite 50% Dahllite
16	70% Whewellite 30% Weddellite	60	60% Whewellite 40% Dahllite
17	80% Whewellite 20% Weddellite	61	70% Whewellite 30% Dahllite
18	90% Whewellite 10% Weddellite	62	80% Whewellite 20% Dahllite
19	90% Uric Acid 10% Whewellite	63	90% Whewellite 10% Dahllite
20	80% Uric Acid 20% Whewellite	64	90% Brushite 10% Whewellite
21	70% Uric Acid 30% Whewellite	65	80% Brushite 20% Whewellite
22	60% Uric Acid 40% Whewellite	66	70% Brushite 30% Whewellite
23	50% Whewellite 50% Uric Acid	67	60% Brushite 40% Whewellite
24	60% Whewellite 40% Uric Acid	68	50% Whewellite 50% Brushite
25	70% Whewellite 30% Uric Acid	69	60% Whewellite 40% Brushite
26	80% Whewellite 20% Uric Acid	70	70% Whewellite 30% Brushite
27	90% Whewellite 10% Uric Acid	71	80% Whewellite 20% Brushite
28	90% Uric Acid Dihydrate 10% Whewellite	72	90% Whewellite 10% Brushite
29	80% Uric Acid Dihydrate 20% Whewellite	73	90% Cystine 10% Whewellite
30	70% Uric Acid Dihydrate 30% Whewellite	74	80% Cystine 20% Whewellite
31	60% Uric Acid Dihydrate 40% Whewellite	75	70% Cystine 30% Whewellite
32	50% Whewellite 50% Uric Acid Dihydrate	76	60% Cystine 40% Whewellite
33	60% Whewellite 40% Uric Acid Dihydrate	77	50% Whewellite 50% Cystine
34	70% Whewellite 30% Uric Acid Dihydrate	78	60% Whewellite 40% Cystine
35	80% Whewellite 20% Uric Acid Dihydrate	79	70% Whewellite 30% Cystine
36	90% Whewellite 10% Uric Acid Dihydrate	80	80% Whewellite 20% Cystine
37	90% Ammonium Hydrogen Urate 10% Whewellite	81	90% Whewellite 10% Cystine
38	80% Ammonium Hydrogen Urate 20% Whewellite	82	90% Uric Acid 10% Weddellite
39	70% Ammonium Hydrogen Urate 30% Whewellite	83	80% Uric Acid 20% Weddellite
40	60% Ammonium Hydrogen Urate 40% Whewellite	84	70% Uric Acid 30% Weddellite
41	50% Whewellite 50% Ammonium Hydrogen Urate	85	60% Uric Acid 40% Weddellite
42	60% Whewellite 40% Ammonium Hydrogen Urate	86	50% Weddellite 50% Uric Acid
43	70% Whewellite 30% Ammonium Hydrogen Urate	87	60% Weddellite 40% Uric Acid
44	80% Whewellite 20% Ammonium Hydrogen Urate	88	70% Weddellite 30% Uric Acid

89 80% Weddellite 20% Uric Acid
 90 90% Weddellite 10% Uric Acid
 91 90% Uric Acid Dihydrate 10% Weddellite
 92 80% Uric Acid Dihydrate 20% Weddellite
 93 70% Uric Acid Dihydrate 30% Weddellite
 94 60% Uric Acid Dihydrate 40% Weddellite
 95 50% Weddellite 50% Uric Acid Dihydrate
 96 60% Weddellite 40% Uric Acid Dihydrate
 97 70% Weddellite 30% Uric Acid Dihydrate
 98 80% Weddellite 20% Uric Acid Dihydrate
 99 90% Weddellite 10% Uric Acid Dihydrate
 100 90% Ammonium Hydrogen Urate 10% Weddellite
 101 80% Ammonium Hydrogen Urate 20% Weddellite
 102 70% Ammonium Hydrogen Urate 30% Weddellite
 103 60% Ammonium Hydrogen Urate 40% Weddellite
 104 50% Weddellite 50% Ammonium Hydrogen Urate
 105 60% Weddellite 40% Ammonium Hydrogen Urate
 106 70% Weddellite 30% Ammonium Hydrogen Urate
 107 80% Weddellite 20% Ammonium Hydrogen Urate
 108 90% Weddellite 10% Ammonium Hydrogen Urate
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 110 80% Struvite 20% Weddellite
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 121 60% Dahllite 40% Weddellite
 122 50% Weddellite 50% Dahllite
 123 60% Weddellite 40% Dahllite
 124 70% Weddellite 30% Dahllite
 125 80% Weddellite 20% Dahllite
 126 90% Weddellite 10% Dahllite
 127 90% Brushite 10% Weddellite
 128 80% Brushite 20% Weddellite
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 591 70% Dahllite 20% Ammonium Hydrogen Urate 10% Whewellite
 592 60% Whewellite 30% Ammonium Hydrogen Urate 10% Dahllite
 593 50% Whewellite 30% Ammonium Hydrogen Urate 20% Dahllite
 594 40% Whewellite 30% Ammonium Hydrogen Urate 30% Dahllite
 595 40% Dahllite 30% Ammonium Hydrogen Urate 30% Whewellite
 596 50% Dahllite 30% Ammonium Hydrogen Urate 20% Whewellite
 597 60% Dahllite 30% Ammonium Hydrogen Urate 10% Whewellite
 598 50% Whewellite 40% Ammonium Hydrogen Urate 10% Dahllite
 599 40% Ammonium Hydrogen Urate 40% Whewellite 20% Dahllite
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 603 50% Ammonium Hydrogen Urate 40% Whewellite 10% Dahllite
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 607 60% Ammonium Hydrogen Urate 30% Whewellite 10% Dahllite
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614 70% Struvite 20% Dahllite 10% Ammonium Hydrogen Urate
615 60% Struvite 30% Dahllite 10% Ammonium Hydrogen Urate
616 50% Struvite 40% Dahllite 10% Ammonium Hydrogen Urate
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618 60% Dahllite 30% Struvite 10% Ammonium Hydrogen Urate
619 70% Dahllite 20% Struvite 10% Ammonium Hydrogen Urate
620 80% Dahllite 10% Ammonium Hydrogen Urate 10% Struvite
621 70% Struvite 20% Ammonium Hydrogen Urate 10% Dahllite
622 60% Struvite 20% Ammonium Hydrogen Urate 20% Dahllite
623 50% Struvite 30% Dahllite 20% Ammonium Hydrogen Urate
624 40% Dahllite 40% Struvite 20% Ammonium Hydrogen Urate
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626 60% Dahllite 20% Ammonium Hydrogen Urate 20% Struvite
627 70% Dahllite 20% Ammonium Hydrogen Urate 10% Struvite
628 60% Struvite 30% Ammonium Hydrogen Urate 10% Dahllite
629 50% Struvite 30% Ammonium Hydrogen Urate 20% Dahllite
630 40% Struvite 30% Ammonium Hydrogen Urate 30% Dahllite
631 40% Dahllite 30% Ammonium Hydrogen Urate 30% Struvite
632 50% Dahllite 30% Ammonium Hydrogen Urate 20% Struvite
633 60% Dahllite 30% Ammonium Hydrogen Urate 10% Struvite
634 50% Struvite 40% Ammonium Hydrogen Urate 10% Dahllite
635 40% Ammonium Hydrogen Urate 40% Struvite 20% Dahllite
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638 50% Dahllite 40% Ammonium Hydrogen Urate 10% Struvite
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645 60% Ammonium Hydrogen Urate 30% Dahllite 10% Struvite
646 70% Ammonium Hydrogen Urate 20% Struvite 10% Dahllite
647 70% Ammonium Hydrogen Urate 20% Dahllite 10% Struvite
648 80% Ammonium Hydrogen Urate 10% Dahllite 10% Struvite
649 80% Struvite 10% Brushite 10% Dahllite
650 70% Struvite 20% Dahllite 10% Brushite
651 60% Struvite 30% Dahllite 10% Brushite
652 50% Struvite 40% Dahllite 10% Brushite
653 50% Dahllite 40% Struvite 10% Brushite
654 60% Dahllite 30% Struvite 10% Brushite
655 70% Dahllite 20% Struvite 10% Brushite
656 80% Dahllite 10% Brushite 10% Struvite
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661 50% Dahllite 30% Struvite 20% Brushite
662 60% Dahllite 20% Brushite 20% Struvite
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664 60% Struvite 30% Brushite 10% Dahllite
665 50% Struvite 30% Brushite 20% Dahllite
666 40% Struvite 30% Brushite 30% Dahllite
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669 60% Dahllite 30% Brushite 10% Struvite
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681 60% Brushite 30% Dahllite 10% Struvite
682 70% Brushite 20% Struvite 10% Dahllite
683 70% Brushite 20% Dahllite 10% Struvite
684 80% Brushite 10% Dahllite 10% Struvite
685 80% Struvite 10% Uric Acid 10% Dahllite
686 70% Struvite 20% Dahllite 10% Uric Acid
687 60% Struvite 30% Dahllite 10% Uric Acid
688 50% Struvite 40% Dahllite 10% Uric Acid
689 50% Dahllite 40% Struvite 10% Uric Acid
690 60% Dahllite 30% Struvite 10% Uric Acid
691 70% Dahllite 20% Struvite 10% Uric Acid
692 80% Dahllite 10% Uric Acid 10% Struvite
693 70% Struvite 20% Uric Acid 10% Dahllite
694 60% Struvite 20% Uric Acid 20% Dahllite
695 50% Struvite 30% Dahllite 20% Uric Acid
696 40% Dahllite 40% Struvite 20% Uric Acid
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698 60% Dahllite 20% Uric Acid 20% Struvite
699 70% Dahllite 20% Uric Acid 10% Struvite
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717 60% Uric Acid 30% Dahllite 10% Struvite
718 70% Uric Acid 20% Struvite 10% Dahllite
719 70% Uric Acid 20% Dahllite 10% Struvite
720 80% Uric Acid 10% Dahllite 10% Struvite
721 80% Ammonium Hydrogen Urate 10% Uric Acid 10% Dahllite
722 70% Ammonium Hydrogen Urate 20% Dahllite 10% Uric Acid

723 60% Ammonium Hydrogen Urate 30% Dahllite 10% Uric Acid
724 50% Ammonium Hydrogen Urate 40% Dahllite 10% Uric Acid
725 50% Dahllite 40% Ammonium Hydrogen Urate 10% Uric Acid
726 60% Dahllite 30% Ammonium Hydrogen Urate 10% Uric Acid
727 70% Dahllite 20% Ammonium Hydrogen Urate 10% Uric Acid
728 80% Dahllite 10% Uric Acid 10% Ammonium Hydrogen Urate
729 70% Ammonium Hydrogen Urate 20% Uric Acid 10% Dahllite
730 60% Ammonium Hydrogen Urate 20% Uric Acid 20% Dahllite
731 50% Ammonium Hydrogen Urate 30% Dahllite 20% Uric Acid
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734 60% Dahllite 20% Uric Acid 20% Ammonium Hydrogen Urate
735 70% Dahllite 20% Uric Acid 10% Ammonium Hydrogen Urate
736 60% Ammonium Hydrogen Urate 30% Uric Acid 10% Dahllite
737 50% Ammonium Hydrogen Urate 30% Uric Acid 20% Dahllite
738 40% Ammonium Hydrogen Urate 30% Uric Acid 30% Dahllite
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740 50% Dahllite 30% Uric Acid 20% Ammonium Hydrogen Urate
741 60% Dahllite 30% Uric Acid 10% Ammonium Hydrogen Urate
742 50% Ammonium Hydrogen Urate 40% Uric Acid 10% Dahllite
743 40% Uric Acid 40% Ammonium Hydrogen Urate 20% Dahllite
744 40% Uric Acid 30% Dahllite 30% Ammonium Hydrogen Urate
745 40% Uric Acid 40% Dahllite 20% Ammonium Hydrogen Urate
746 50% Dahllite 40% Uric Acid 10% Ammonium Hydrogen Urate
747 50% Uric Acid 40% Ammonium Hydrogen Urate 10% Dahllite
748 50% Uric Acid 30% Ammonium Hydrogen Urate 20% Dahllite
749 50% Uric Acid 30% Dahllite 20% Ammonium Hydrogen Urate
750 50% Uric Acid 40% Dahllite 10% Ammonium Hydrogen Urate
751 60% Uric Acid 30% Ammonium Hydrogen Urate 10% Dahllite
752 60% Uric Acid 20% Dahllite 20% Ammonium Hydrogen Urate
753 60% Uric Acid 30% Dahllite 10% Ammonium Hydrogen Urate
754 70% Uric Acid 20% Ammonium Hydrogen Urate 10% Dahllite
755 70% Uric Acid 20% Dahllite 10% Ammonium Hydrogen Urate
756 80% Uric Acid 10% Dahllite 10% Ammonium Hydrogen Urate



Appendix B — Example Spectral Files

This section provides a listing of 212 spectral data files from real kidney stones (found in human kidneys) that are included with the Kidney Stone Library and Analysis Software. The spectra are listed by file name. A descriptive compound name appears to the right of each file name. These example spectra typically are stored in the \Kidstone\Kidstone_Spectra_Examples\ directory.

The software also includes 23 spectral files from pure chemical compounds that represent the primary components found in typical kidney stones. You can use these example spectra to try out the various features of the Kidney Stone Library and Analysis Software and to duplicate the procedures that are described in this manual.

File Name Compound Description

kidst001	Xanthine and Sodium urate monohydrate	kidst028	Dahllite
kidst002	Paraffin	kidst029	Weddellite
kidst003	Gypsum	kidst030	Struvite and Amorphous calcium phosphate-carbonate
kidst004	Calcite	kidst031	Struvite, Weddellite and Amorphous calcium phosphate-carbonate
kidst005	Uric acid and Whewellite	kidst032	Struvite, Dahllite and Amorphous calcium phosphate-carbonate
kidst006	Cholesterol	kidst033	Weddellite and Brushite
kidst007	Struvite	kidst034	Weddellite and Whewellite
kidst008	Struvite	kidst035	Protein
kidst009	Cystine	kidst036	Dahllite and Whewellite
kidst010	Uric acid	kidst037	Ammonium urate and Uric acid
kidst011	Uric acid and Weddellite	kidst038	Dahllite and Whitlockite
kidst012	Dahllite, Weddellite and Amorphous calcium phosphate-carbonate	kidst039	Dahllite, Whewellite and Weddellite
kidst013	Whewellite and Weddellite	kidst040	Dahllite and Weddellite
kidst014	Uric acid and Whewellite	kidst041	Weddellite, Whewellite and Cystine
kidst015	Sodium urate monohydrate, Weddellite and Ammonium urate	kidst042	Dahllite and Whitlockite
kidst016	Whewellite and Brushite	kidst043	Calcite
kidst017	Cholesterol	kidst044	Uric acid and Whewellite
kidst018	N4-Acetylsulfamethoxazole	kidst045	Whewellite
kidst019	Whewellite	kidst046	Struvite and Ammonium urate
kidst020	2,8-dihydroxyadenine	kidst047	Dahllite, Whewellite and Weddellite
kidst021	Uric acid and Weddellite	kidst048	Dahllite and Whewellite
kidst022	Weddellite and Whewellite	kidst049	Dahllite and Ammonium urate
kidst023	Weddellite and Uric acid	kidst050	Uric acid
kidst024	Weddellite and Uric acid	kidst051	Ammonium urate, Newberyite and Uric acid
kidst025	Dahllite, Whitlockite and Struvite	kidst052	Uric acid
kidst026	Weddellite	kidst053	Struvite, Dahllite and Ammonium urate
kidst027	Uric acid	kidst054	Uric acid

kidst055 Sodium urate, Dahllite and Weddellite
 kidst056 Uric acid and Ammonium urate
 kidst057 Uric acid and Whewellite
 kidst058 Unknown
 kidst059 Oxolinic acid
 kidst060 Calcite
 kidst061 Struvite, Dahllite and Ammonium urate
 kidst062 Whewellite and Weddellite
 kidst063 Indigo
 kidst064 Bee's wax
 kidst065 Aragonite
 kidst066 Gypsum
 kidst067 Dahllite
 kidst068 Whewellite and Weddellite
 kidst069 Gypsum
 kidst070 Calcite
 kidst071 alpha-Quartz
 kidst072 Uric acid
 kidst073 Whewellite
 kidst074 Whewellite
 kidst075 Whewellite and Weddellite
 kidst076 Uric acid and Ammonium urate
 kidst077 Weddellite and Whewellite
 kidst078 Weddellite
 kidst079 Whewellite and Weddellite
 kidst080 Whewellite
 kidst081 Dahllite, Struvite and Amorphous calcium phosphate-carbonate
 kidst082 Weddellite and Dahllite
 kidst083 Whewellite
 kidst084 Uric acid
 kidst085 Struvite, Dahllite and Amorphous calcium phosphate-carbonate
 kidst086 Uric acid and Whewellite
 kidst087 Weddellite and Whewellite
 kidst088 Weddellite, Whewellite and Amorphous calcium phosphate-carbonate
 kidst089 Uric acid
 kidst090 Weddellite and Whewellite
 kidst091 Weddellite, Whewellite and Dahllite
 kidst092 Struvite, Dahllite and Amorphous calcium phosphate-carbonate
 kidst093 Weddellite and Whewellite
 kidst094 Dahllite, Whewellite and Weddellite
 kidst095 Weddellite
 kidst096 Uric acid
 kidst097 Uric acid
 kidst098 Whewellite and Weddellite
 kidst099 Uric acid
 kidst100 Whewellite and Weddellite
 kidst101 Whewellite and Weddellite
 kidst102 Uric acid
 kidst103 Dahllite and Whewellite
 kidst104 Whewellite and Weddellite
 kidst105 Whewellite and Weddellite
 kidst106 Weddellite and Whewellite
 kidst107 Whewellite and Weddellite
 kidst108 Newberyite, Amorphous calcium phosphate-carbonate and Ammonium urate
 kidst109 Weddellite and Dahllite
 kidst110 Whewellite
 kidst111 Oxolinic acid
 kidst112 Whewellite and Uric acid
 kidst113 Whewellite and Uric acid
 kidst114 Uric acid and Weddellite
 kidst115 Dahllite and Weddellite
 kidst116 Struvite and Amorphous calcium phosphate-carbonate
 kidst117 Whewellite and Amorphous calcium phosphate-carbonate
 kidst118 Uric acid
 kidst119 Whewellite
 kidst120 Uric acid and Whewellite
 kidst121 Ammonium urate and Uric acid
 kidst122 Uric acid
 kidst123 Struvite and Dahllite
 kidst124 Dahllite and Amorphous calcium phosphate-carbonate
 kidst125 Dahllite and Wheddellite
 kidst126 Dahllite and Struvite
 kidst127 Dahllite
 kidst128 Struvite, Dahllite and Amorphous calcium phosphate-carbonate
 kidst129 Dahllite, Ammonium urate and Wheddellite
 kidst130 Struvite, Dahllite and Amorphous calcium phosphate-carbonate
 kidst131 Brushite
 kidst132 Brushite and Weddellite
 kidst133 Ammonium urate and Sodium urate monohydrate
 kidst134 Ammonium urate and Sodium urate monohydrate
 kidst135 Ammonium urate and Uric acid
 kidst136 Ammonium urate, Sodium urate monohydrate and Weddellite
 kidst137 Uric acid
 kidst138 Uric acid and Weddellite
 kidst139 Uric acid and Weddellite
 kidst140 Uric acid
 kidst141 Uric acid
 kidst142 Uric acid
 kidst143 Uric acid
 kidst144 Uric acid
 kidst145 Uric acid
 kidst146 Dahllite
 kidst147 Dahllite and Struvite
 kidst148 Uric acid and Whewellite
 kidst149 Dahllite
 kidst150 Whewellite
 kidst151 Uric acid and Weddellite
 kidst152 Uric acid and Weddellite
 kidst153 Ammonium urate and Weddellite
 kidst154 Cystine
 kidst155 Ammonium urate and Whewellite
 kidst156 Brushite
 kidst157 Ammonium urate and Sodium urate monohydrate
 kidst158 Brushite and Weddellite
 kidst159 Uric acid and Whewellite
 kidst160 Whewellite and Cystine
 kidst161 Whewellite and Weddellite
 kidst162 Struvite, Ammonium urate and Amorphous calcium phosphate-carbonate
 kidst163 Ammonium urate and Weddellite

kidst164 Ammonium urate, Sodium urate monohydrate and Weddellite
kidst165 Uric acid
kidst166 Furantoinine
kidst167 Whewellite and Weddellite
kidst168 Calcite
kidst169 Whewellite and Weddellite
kidst170 Brushite and Weddellite
kidst171 Struvite and Newberyite
kidst172 Sodium urate monohydrate and Whewellite
kidst173 Xanthine and Weddellite
kidst174 Albite, Kaolinite and alpha-Quartz
kidst175 Brick fragment
kidst176 Cholesterol
kidst177 Calcite
kidst178 Gypsum
kidst179 Paraffin
kidst180 Aragonite
kidst181 Oxolinic acid
kidst182 Calcite
kidst183 Dahllite and Whitlockite
kidst184 N4-acetylsulfamethoxazole
kidst185 Newberyite
kidst186 Brick fragment
kidst187 Weddellite

kidst188 Uric acid
kidst189 Uric acid and Weddellite
kidst190 Uric acid and Weddellite
kidst191 Sodium urate monohydrate and Whewellite
kidst192 Uric acid and Weddellite
kidst193 Cysteine
kidst194 alpha-Quartz
kidst195 Gypsum
kidst196 Indigo
kidst197 2,8-dihydroxyadenine
kidst198 Cystine
kidst199 Uric acid
kidst200 Ammonium urate
kidst201 Weddellite
kidst202 Uric acid
kidst203 Brushite
kidst204 Struvite
kidst205 Dahllite, Whitlockite and Struvite
kidst206 Whewellite
kidst207 Sodium urate monohydrate and Ammonium urate
kidst208 Uric acid
kidst209 Struvite
kidst210 Xanthine
kidst211 Dahllite, Whitlockite and Struvite
kidst212 Weddellite



Appendix C — The Coded Library

In some cases it might be useful to use the coded library directly as a spectral library (using the SEARCH function of your OMNIC software). The coded library is located in the same directory as the Kidney Stone Analysis Kit files or on the installation CD in directory "Kidstone files". Select the correct library path in OMNIC software and compare (SEARCH) your spectrum to the library spectra. The spectra in the coded library have coded titles, use the following table to decode the titles. The component number is identical with the number of pure component spectrum used for the visual comparison.

<i>No.</i>	<i>Component</i>	<i>No.</i>	<i>Component</i>
0	"Whewellite"	13	"2,8 - dihydroxyadenine"
1	"Weddellite"	14	"Hydroxylapatite"
2	"Cystine"	15	"Calcite"
3	"Xanthine"	16	"Aragonite"
4	"Proteine"	17	"Gypsum"
5	"Dahllite"	18	"alpha - Quartz"
6	"Struvite"	19	"Tridymite"
7	"Brushite"	20	"N4 -
8	"Uric acid"	21	"Oxolinic acid"
9	"Uric acid dihydrate"	22	"Cholesterol"
10	"Ammonium urate"	23	"Whitlockite"
11	"Sodium urate monohydrate"	24	"Newberyite"
12	"Calcium phosphate"	25	"Potassium urate"

Example of Search result 2 0 30 1 70

1. number (2) - number of components
2. number (0) - code number of first component (Whewellite)
3. number (30) - percentage of first component (Whewellite)
4. number (1) - code number of second component (Weddellite)
5. number (70) - percentage of second component (Weddellite)

Three component mixtures have the analogous coding.