

Getting the Most from Your Sample Data with the Agilent 8700 LDIR Chemical Imaging System

Data management and analysis options for microplastic analysis



Introduction

Microplastics have gained significant attention in the field of environmental analysis as the threats associated with their contamination of soil, air, and water are more fully understood. Chemical identification, number, size, and shape of microplastics are key characteristics that researchers look for in analytical samples. Given the diversity of these characteristics, streamlined, easy-to-use, and hands-off analytical software is key for high-throughput sample analysis. The amount of data generated during an analysis is also highly dependent on the matrix and, in some cases, the data from multiple thousands of particles will be collected and stored. As microplastic analysis becomes more established, being able to manage the large amount of data and images generated from a regular analysis is becoming increasingly important.

The **Agilent 8700 LDIR Chemical Imaging System** and **Agilent Clarity software** together provide users with a fast, automated workflow that locates, images, measures, and identifies microplastics without the need to export data to other external software or perform extra analyses. This means that samples can be analyzed and understood even by users who are new to the software or have little understanding of spectroscopic techniques. Clarity software also provides options to examine results in more detail where a deeper understanding is required, and it provides a straightforward archiving process that allows users to store and move their data to a data storage location of their choice. This technical overview describes how Clarity software presents its data, and the options available to users for further analysis and data storage.

Particle analysis results at a glance

Once the particle analysis is complete, Clarity software presents the results in an easy-to-parse format, giving the user immediate information about the most important aspects of their sample without the need for further processing.

Particle data

Clarity software displays an overview of each particle in the Particles tab of the Particle Analysis panel (Figure 1). This gives detailed information, including:

- Number of particles
- Visible and IR images
- Chemical identification
- Collected spectra overlaid on library matches
- Hit quality index (HQI)
- Size information

In this tab, the user may also choose to include or remove individual particles from statistical data and add particle-specific notes.

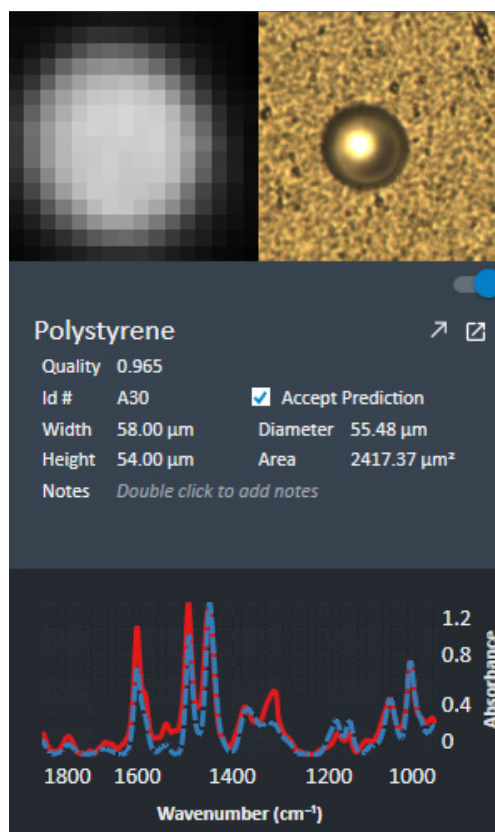


Figure 1. Particle data in the Particle Analysis panel.

Identifications breakdown

A histogram of the particle identification results is displayed on the Identifications tab (Figure 2). The data available here are:

- An ordered histogram of the most-to-least-common identifications
- The percentage of each identification
- The number of particles of each identification

The user may also choose to highlight the particles on the image with solid colors to provide a visual representation of the spatial distribution of particle identifications across the sample.

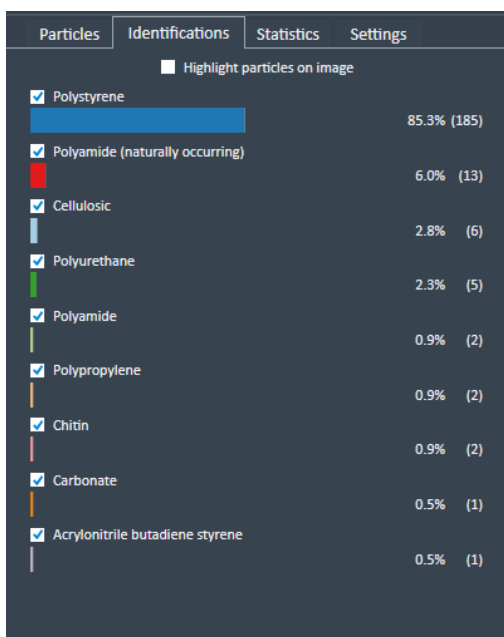


Figure 2. Identifications breakdown.

Particle diameter distribution

A histogram of the particle diameter distribution is displayed on the Statistics tab (Figure 3). The particle counts can be displayed discretely or in user-customizable buckets. Users can customize which particle identifications are displayed on the histogram, allowing the diameter distribution of specific particle types to be viewed.

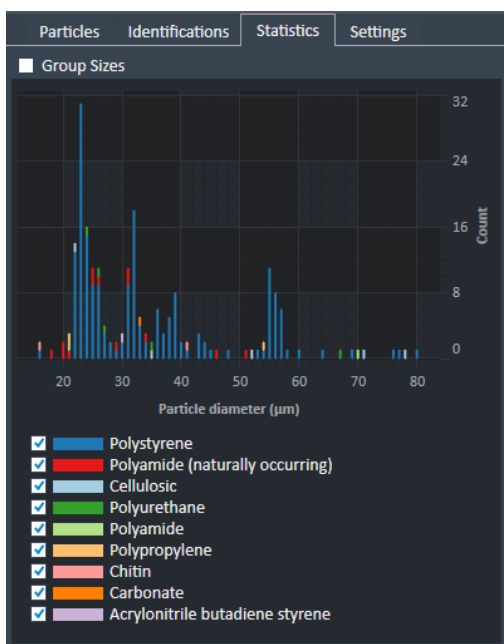


Figure 3. Statistics tab showing the particle diameter distribution.

Particle spectra

The Spectral Viewer window displays every spectrum collected during the particle analysis and automatically names the spectra to associate them with their respective particles. In this window (Figure 4), the collected spectra may be compared and matched to library spectra, viewed in multiple resolutions, mathematically transformed, and compared, averaged, and subtracted from other collected spectra.

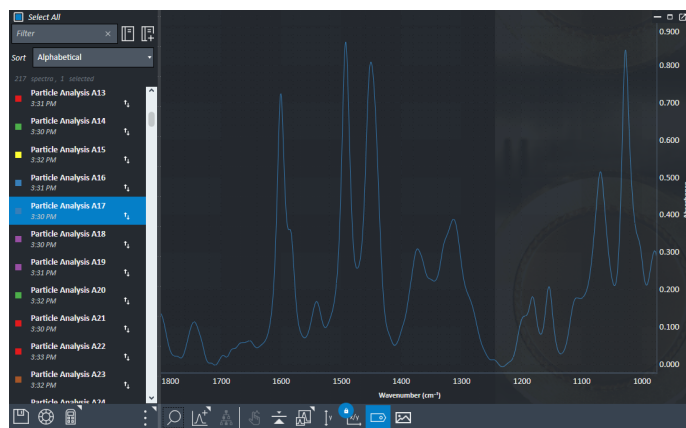


Figure 4. Spectral Viewer window.

Getting the most out of your sample data

Once the particle analysis data have been collected, there are options to reanalyze it within Clarity software. This can be done on either the PC connected to the instrument or on a different PC via the Clarity Viewer application that is available automatically when Clarity software is installed. Exported data files can be imported into any other Clarity installations and viewed in the same way as on the instrument PC.

Reanalysis

When a particle analysis identifies particles, it does so against a single library of spectra. If users would like to match their collected particles against an updated or completely different library, they may do so by reanalyzing a method. This will create a new method and use the newly selected library to match every particle in the method again. For further information on this feature, see this [application note](#).

Customized matching

The particle analysis workflow will automatically attribute a single identification with the highest HQI to each particle. However, users also have the option to look at the top five matches from any imported library and manually assign that match to the particle. This particle will then be tagged as a user-defined particle match in both the Clarity results window and any exported results (Figure 5).

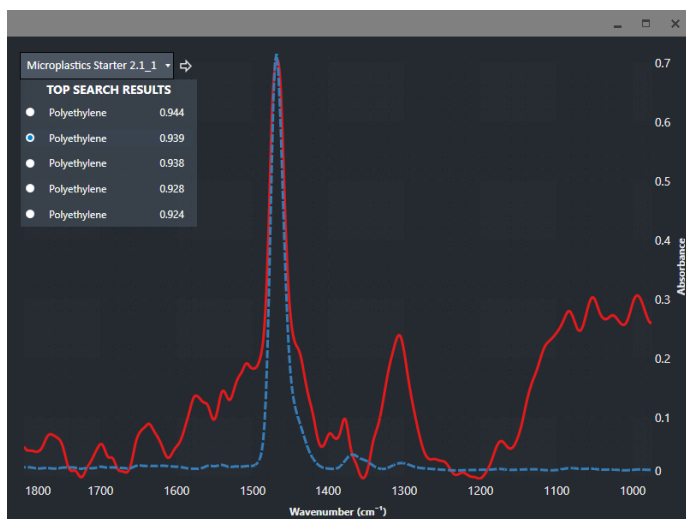


Figure 5. User definition of particle identification.

Exporting and archiving samples

Clarity software stores data in a format that combines a database and software-specific spectra files. To manage these data, users can use the Export and Archive functionalities provided on the Clarity Home page (Figure 6). Exporting samples will create files that can be imported into instances of Clarity software on other PCs to allow further viewing and analysis of results outside of the laboratory.

Archiving will export single or multiple samples at a time and then delete them from the Clarity Home page and the Clarity data folder. This is useful for ensuring that the Clarity data drive does not fill up, and it allows users to use their own secure storage solutions. Samples will be archived individually and labeled with their sample names; so, if the data need to be retrieved and viewed later, samples can be imported back into Clarity software on the same or other PCs. The length of time to archive a sample will be determined by the size of the sample. In general, a 1 GB sample file (representing data from approximately 5,000 particles) will take 30 minutes to archive.

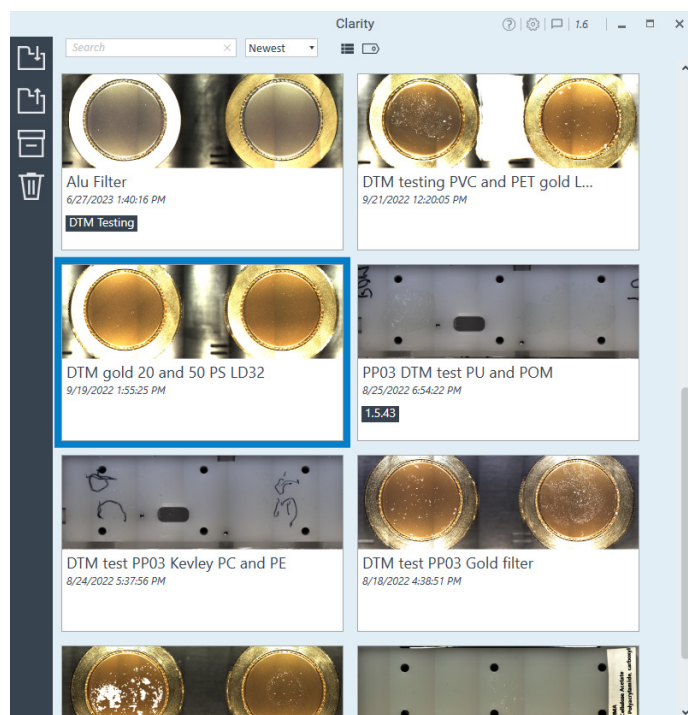


Figure 6. Clarity Home window for sample management.

When viewing and analyzing samples on non-instrument PCs, it is recommended that the PC specifications are roughly equivalent to those given in Table 1.

Table 1. Suggested PC specifications for data analysis.

Specification	Recommendation
RAM	32 GB
CPU	3.60 GHz
Graphics Card	Dedicated GPU recommended

Exporting data to other formats

If further reprocessing or a specific data presentation style is required, Clarity software allows users to export particle data, images, and spectra in various common formats.

Particle data

Particle data from each analysis method can be exported from the Particle tab of the method window. This will generate either a Microsoft Excel or CSV formatted file that includes particle names, identification, hit quality, size data, and notes. These data include results required by methods published or under development such as **ISO/DIS 16094-2 Water Quality: Analysis of Microplastic in Water** and the Policy Handbook for Testing and Reporting Microplastics in Drinking Water published by **California Water Boards**.

Images

The high-resolution IR image generated to find the particles (Figure 7) can be saved in multiple formats including png, CSV, envi, and PDF. The image can be saved without any additions, with boundaries drawn around the identified particles or with all particles highlighted and colored. IR and high-magnification visible images of each individual particle can be exported simply by selecting the **Save Images check box** in the Settings tab and exporting the particle data. This will generate a folder with both the exported particle data and images for each particle, labeled with the particle ID number.

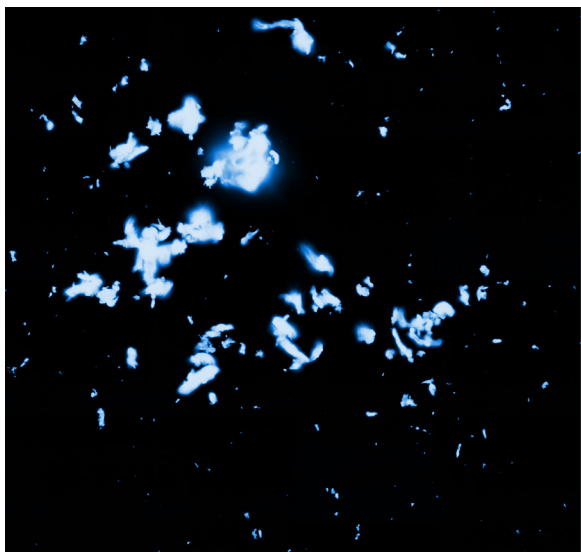


Figure 7. IR image used for particle finding.

Spectra

Particle spectra can be exported as a CSV or Excel spreadsheet for further analysis. Exporting multiple spectra in this way will create a single Excel spreadsheet with two columns (wavenumber and intensity) for each spectrum. Images of the spectra can also be saved easily from the Spectral Viewer window (Figure 8).

Bio-Rad

Clarity software features the ability to automatically import spectral data from a particle analysis or the spectral viewer to Bio-Rad Laboratories KnowItAll analytical software.

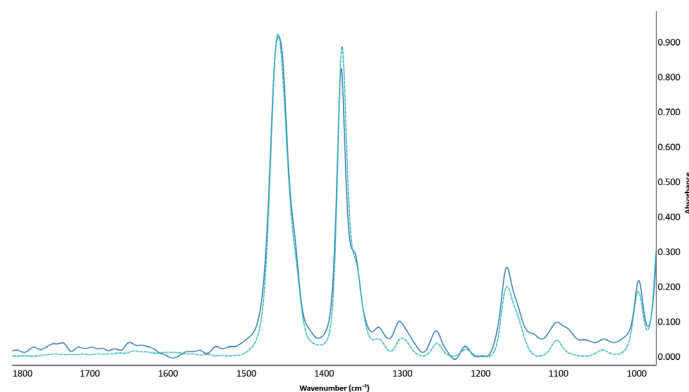


Figure 8. Image of collected spectrum saved from the Spectral Viewer window.

Conclusion

The Agilent 8700 LDIR chemical imaging system and Agilent Clarity software provide an end-to-end, fully automated workflow for detecting and identifying microplastics. The data generated by this workflow are also presented to the user in a clear and readily available format that meets the requirements of existing and emerging standardized testing methodology, meaning samples can be understood in an instant, even by users without a spectroscopic background. Equally important is the ability to manage the large amount of data that is typically generated by microplastic analysis. Clarity provides intuitive data archiving and export options, which allow samples and sample data to be transferred from the instrument PC to user-defined secure storage locations for further analysis or to free up storage space. If further analysis is required, Clarity data can be exported in various common formats. The 8700 LDIR makes the analysis of microplastics fast, easy, and effective.

Further information

- [Agilent 8700 LDIR Chemical Imaging System](#)
- [Agilent Clarity Software](#)
- [Microplastics Technologies FAQs](#)
- [Microplastics Analysis in Water](#)

www.agilent.com/chem/8700-lidir

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