

iSpect DIA – Shimadzu

INTRODUCTION

The Lumetics LINK™ software platform scans network locations for new measurement data files, copies data directly to a centralized database, and provides a powerful user interface for rapid multi-measurement multi-technique data aggregation, visualization, analysis, and reporting. LINK employs a client/server-based architecture where the LINK server hardware is provided by the end user and resides on the end user's network. The LINK client is a portable web-based application that may be placed on any computer with network connectivity to the LINK server. For successful import, the LINK webserver requires read access to the folders where user data resides.

Shimadzu's iSpect DIA-10 Dynamic Image Analyzer combines particle size and image analysis technology to offer complete particle characterization. It can perform particle imaging, size analysis, and foreign object detection, and obtain size distributions and number concentration.

DETAILS

LINK requires the run-level summary SDAT generated automatically by the iSpect DIA system. When utilized, data outside the specified acceptance range will not be imported. Particle images may optionally be imported as JPGs, and therefore may be exported as thumbnail images from LINK as JPGs.

Particle count/concentration for each supported morphological parameter occurs at a pre-defined bin spacing and measurement range as per the table below. Default measurement ranges will dynamically widen based as required, based on the datasets imported to LINK.

Parameter Name	Bin Spacing	Meas. Start	Meas. End
Particle Diameter (µm)	0.25	0	2500
Perimeter Based Diameter (µm)	0.25	0	2500
Max Distance	0.25	0	2500
Min Distance	0.25	0	2500
Max Feret Diameter (µm)	0.25	0	2500
Min Feret Diameter (µm)	0.25	0	2500
Length	0.25	0	2500
Horizontal Feret Diameter (µm)	0.25	0	2500
Vertical Feret Diameter (µm)	0.25	0	2500
Perimeter	1	0	1000
Cperimeter	1	0	1000
Area	1	0	1000
Circularity	0.01	0	1
Circular Degree Based Area	0.01	0	1
Aspect Ratio	0.01	0	1
Aspect Ratio (ISO)	0.01	0	1
Box Ratio (ISO)	0.01	0	10
Feret Aspect Ratio	0.01	0	1



Intensity Mean	1	0	255
Intensity Maximum	1	0	255
Intensity Minimum	1	0	255
Intensity Standard Deviation	1	0	255
Compactness (ISO)	0.01	0	5
Roundness (ISO)	0.01	0	5
Convexity (ISO)	0.01	0	1
Extent (ISO)	0.01	0	5
Geodesic Length (ISO)	0.25	0	2500
Geodesic Thickness (ISO)	0.25	0	2500
Straightness (ISO)	0.01	0	5
Elongation (ISO)	0.01	0	5
Edge Gradient	1	0	2500

The iSpect DIA data file example is as follows:

```

1  <?xml version="1.0" encoding="shift_jis"?>
2  <datResult xmlns:xsd="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
3    <VERS>0.0</VERS>
4    <PROG />
5    <START_DATE>2021/09/30 15:23:38</START_DATE>
6    <END_DATE>2021/09/30 15:28:38</END_DATE>
7    <RECALC_DATE />
8    <S_ID>standard_CC15</S_ID>
9    <S_NO>7</S_NO>
10   <INSTRUMENT_METHOD>20210930_Standards_AL</INSTRUMENT_METHOD>
11   <DATA_METHOD>20210930_Standards_AL</DATA_METHOD>
12   <OUTPUT_METHOD>20210930_Standards_AL</OUTPUT_METHOD>
13   <COMMENT />
14   <SYSTEMINFO>
15     <SingleMethod>20210930_Standards_AL</SingleMethod>
16     <EmissionIntensity />
17     <Clipping_X>200</Clipping_X>
18     <Clipping_Y>0</Clipping_Y>
19     <Clipping_Width>2048</Clipping_Width>
20     <Clipping_Height>1100</Clipping_Height>
21     <ClippingON>1</ClippingON>
22     <MaxFrameCount>0</MaxFrameCount>
23     <ThumbnailMargin>15</ThumbnailMargin>
24     <DifferenceImage>0</DifferenceImage>
25     <LEDControl>0</LEDControl>
26     <LEDPower>123</LEDPower>

```

Import Method options can be defined and calculated each measurement during import if it is first created/defined and then requested within an Import Method. More information and instructions can be found in the Users Manual (section 4.27). The following is the default Protein Thermal Shift-specific import method settings:

- Default Sub-Populations: **None**
- Custom Particle Parameters: **None**
- Container Fill Volume: **None**
- Include Edge Particles: **No**
- Number of Thumbnails to Crop: **250**
- Ignore Thumbnails less than: **5 µm**
- Import Images in order of Largest-to-Smallest: **Yes**
- Advanced Metadata Extraction: **None**
- Automated Metadata Extraction: **None**
- Dilution Factor: **1 (no dilution)**

Subpopulations

In addition to the total particle population data set, sub-populations based morphological parameter filters may be generated at the point of measurement import. An unlimited number of sub-populations may be specified for each measurement. For each sub-population, the particle count/concentration vs. morphological parameter will be available, as well as representative particle thumbnail images. The sub-populations do not count towards the measurement limit per project. Additional Sub-Populations will affect import speeds.

When creating as sub-population, select a Morphological Parameter from the pre-defined list and specify the filter criteria. Select the + to add the filter term to the Live Expression View. The Live Expression View can be edited directly. Brackets, mathematical operators/values, logical ANDs or ORs are valid operators. Syntax must be exact, for successful application.



Custom particle Parameters

Select from the available user-defined Custom Particle Parameters, those that shall be calculated for each individual particle within each measurement. This selection applies to the total particle population and all defined sub-populations.

Container Fill Volume

Specify the Container Fill Volume, permitting LINK to calculate and report Particles per Container (in addition to Particle Count, and Particle Concentration). This selection applies to the total particle population and all defined sub-populations.

Edge Particles

Include or exclude Edge particles (particles intersecting the edge of the image frame). This selection applies to the total particle population and all defined sub-populations.

Thumbnail Images

Specify the maximum number of particle thumbnail images to be imported to the LINKdb for each measurement population. Apply a size threshold (the default is 5 microns). Choose whether particles should be first sorted from largest to smallest (based on ECD) or imported in their order of appearance during the analysis. These selections apply to the total particle population and all defined sub-populations.

Advanced Image Selection Criteria: Specify the number of thumbnail images for various particle parameter ranges of interest. The total number of images may not exceed 5000.

Automated Metadata Extraction

Specify criteria for automated metadata extraction from measurement file fields (e.g., Comments, File Name, Import Path etc...) utilizing specified delimiters. Both metadata name and value may be extracted or only the value only.

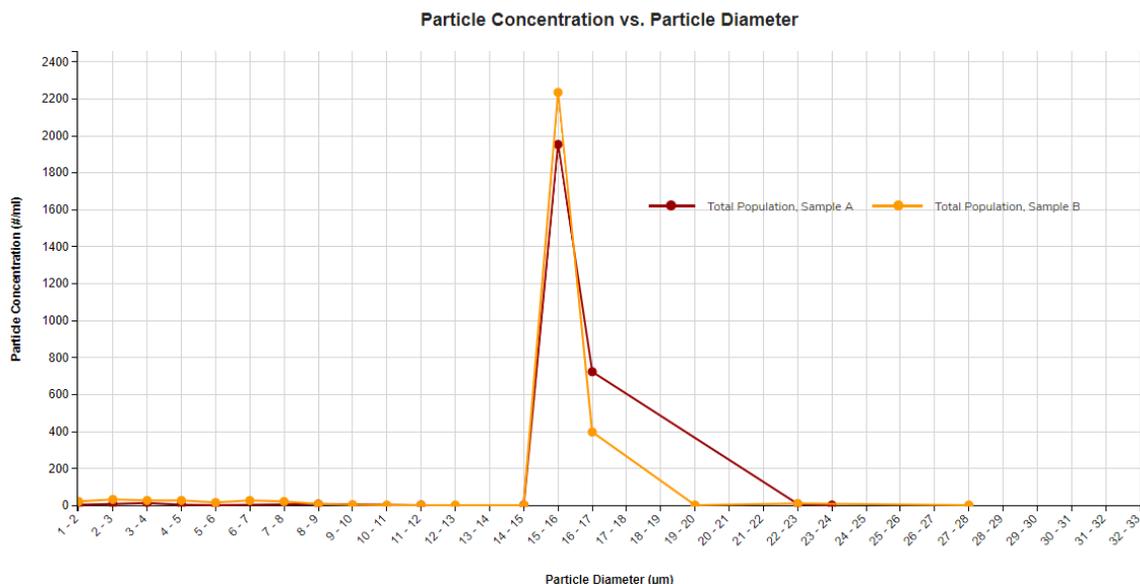
Dilution Factor

Specify a dilution factor for automated particle count/concentration data adjustment. This selection applies to the total particle population and all defined sub-populations. An **LNK_Dilution_Factor** may also be applied after import, utilizing the **Add/Edit LINKdb Fields** feature.

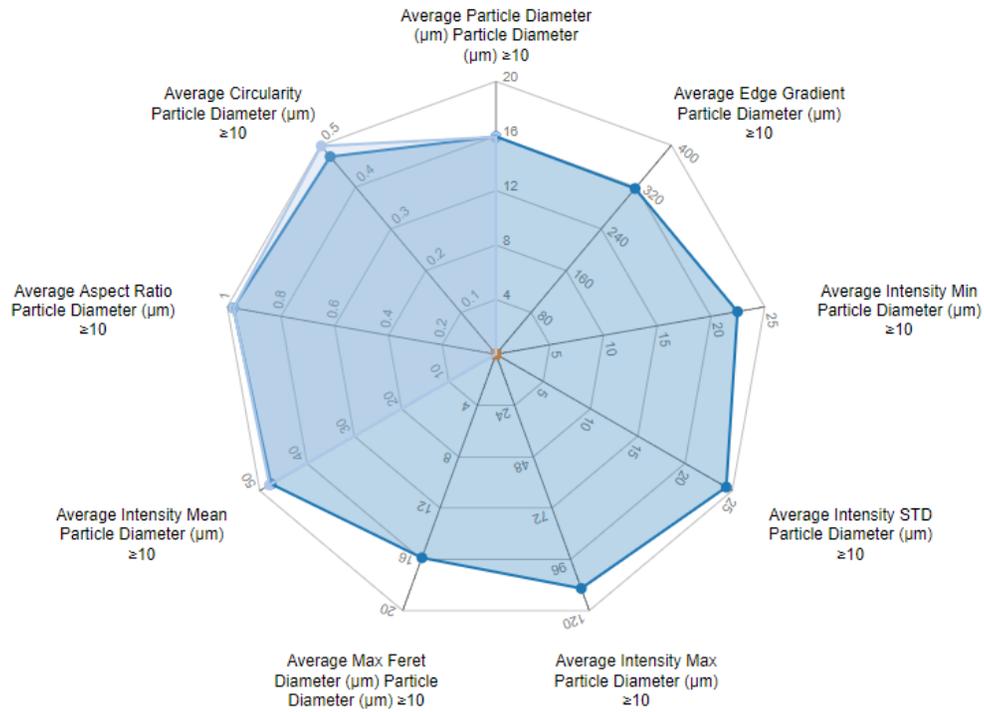
EXAMPLES

Included below are example dashboards from iSpect DIA measurement files:

1. Line Chart plotting raw data based on particle concentration vs. diameter



2. Radar Chart plotting multiple morphological parameters



3. Tabular Summary examples - Measurement Summary Table

Sample Name	Sub-Population	# Meas	Total Count (#)	Total Conc. (#/ml)	1-2µm (#/ml)	2-5µm (#/ml)	5-10µm (#/ml)	$\geq 10\mu\text{m}$ (#/ml)	$\geq 25\mu\text{m}$ (#/ml)	$\geq 50\mu\text{m}$ (#/ml)	$\geq 100\mu\text{m}$ (#/ml)
Sample A	Total Population	1	991	2,738	6	28	11	2,693	0	0	0
Sample B	Total Population	1	1,032	2,851	22	88	80	2,660	3	0	0
Sample C	Total Population	1	0	0	0	0	0	0	0	0	0

CONTACT LUMETICS

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