MicroCal PEAQ-DSC – Malvern Panalytical

INTRODUCTION

The Lumetics LINK^TM 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.

MicroCal ITC (isothermal titration calorimeters) are used to study a wide range of biomolecular interactions. The applications range from drug design to fundamental research such as the understanding and regulation of signal transduction pathways.

DETAILS

LINK can import data from the CSV table export files (with optional curve CSV data and full PDF report as a series attachment), or from the PDF file itself. Importing from the PDF only, will only import table values from the report. To obtain full curve data, import using the table/curve CSV files.

Helpful Notes:

- Fitted data must include a space (seen as a delimiter) then the word "Fit", "Fitted", or "Fitting" as the last word in the record Name for it to be distinguished from the Raw data. Please see examples below:
    - o   Table data csv: Lumetics MicroCal Example_1[13] Fitting
    - o   Raw data csv: Lumetics MicroCal Example_1[13] Fitting – Raw_X
- If both Raw and Fitted data is exported to CSV, LINK will bring both in for comparison/overlay.
- A field called "Measurement Type" will automatically be created, populated, and added to the Analysis Template Filter Panel to denote the curve types.
- Although the 'cell' is not required within the 'Name' column for the table CSV when exporting the data from the MicroCal PEAQ system, please do not remove it. The cell number can help distinguish any sample replicates and therefore prevent skipping non true duplicates at point of import. LINK will automatically strip the cell number from the sample name upon import and applied to a new field called "Cell".
- There are many different variations of the MicroCal PEAQ data exports. Below are the possible scenarios and outcomes:
    - o   If Sample Names are different, we should see all measurements and all curves and peak fits import:
        - ▪   Scenario 1: Table has cell in Raw and cell in Fitted, Curve has cell
        - ▪   Scenario 2: Table has cell in Raw and no cell in Fitted, Curve has cell
        - ▪   Scenario 3: Table has cell in Raw and cell in Fitted, Curve has no cell
        - ▪   Scenario 4: Table has cell in Raw and no cell in Fitted, Curve has no cell

    - o   If the Sample Names are the same, then:
        - ▪   Scenario 1 will import all measurements and curves
        - ▪   Scenario 2 will import only ONE fitted measurement and curve
        - ▪   Scenario 3 will import all measurements and NO curves
        - ▪   Scenario 4 will import only ONE fitted measurement and NO curves

The MicroCal PEAQ CSV data file example is as follows:

	A	B	C	D	E	F	G	H
1	Name	Total Area (kcal/mole)	Tm1 (°C)	Tm2 (°C)	Tm3 (°C)	Tm4 (°C)	Tm5 (°C)	Tm6 (°C)
2	LINK LIMS 2022_rep1[13]	942.165963	70.18	76.64	60.24	N/A	N/A	N/A
3	LINK LIMS 2022_rep2[15]	949.998267	70.19	76.73	72.02	N/A	N/A	N/A
4	LINK LIMS 2022_rep3[17]	950.332217	70.2	76.81	68.09	N/A	N/A	N/A
5	LINK LIMS 2022_rep1[13] - Fitting	942.165963	70.18	76.64	60.24	N/A	N/A	N/A
6	LINK LIMS 2022_rep2[15] - Fitting	949.998267	70.19	76.73	72.02	N/A	N/A	N/A
7	LINK LIMS 2022_rep3[17] - Fiting	950.332217	70.2	76.81	68.09	N/A	N/A	N/A

EXAMPLES

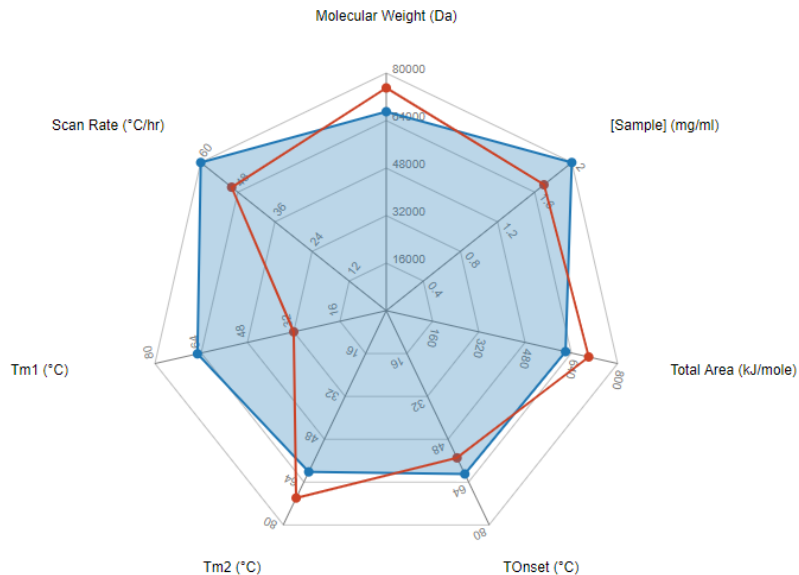Included below are sample dashboards from MicroCal PEAQ measurement files:

1. Line Chart plotting data for Cp vs. Temperature raw data curves
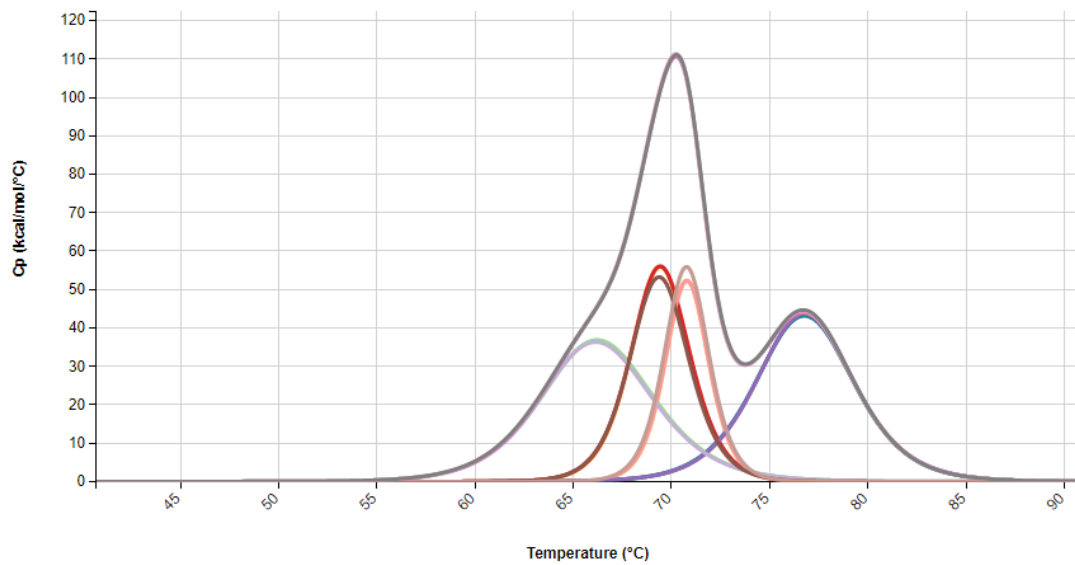
2. Radar Chart plotting multiple parameters with limit lines/acceptance mask

3. Tabular Summary examples:

Measurement Summary Table – Measurement Results

Operator	Scan Rate (°C/hr) - AVG	Tm1 (°C) - AVG	Tm2 (°C) - AVG	Tm3 (°C)	Total Area (kJ/mole) - AVG
Sample A	60	63.29	69.89		
Sample B	60	50.00	79.00	86.49"	620
Sample C	60	58.00	69.89	86	620
Sample D	60	62.00	40.00		
Sample F	60	75.00	38.00	86.49"	620
Sample G	60	79.00	69.89	86	620
Sample H	60	69.77	55.00		

Measurement Summary Table – Instrument Settings

LINK Record ID #	Sample Name	Operator	File Name	Analysis Date	Analysis Software Version - AVG	Instrument Serial Number	Measurement Software Version - AVG	Software Version
1	BSA	Sample A	Link1.pdf	2020-02-19 11:29:00	1.40	MAL1205435	1.40	MicroCal PEAQ-DSC...
2	BSA[2]	Sample B	Link2.pdf	2020-02-19 11:29:00	1.40		1.40	
5	BSA[2]	Sample C	Link2.pdf	2020-02-19 11:29:00	1.40	MAL1205435	1.40	MicroCal PEAQ-DSC...
10	BSA	Sample D	Link1.pdf	2020-02-19 11:29:00	1.40	MAL1205435	1.40	MicroCal PEAQ-DSC...
11	BSA[2]	Sample F	Link2.pdf	2020-02-19 11:29:00	1.40		1.40	
12	BSA[2]	Sample G	Link2.pdf	2020-02-19 11:29:00	1.40	MAL1205435	1.40	MicroCal PEAQ-DSC...
15	BSA	Sample H	MultiDataReport.pdf	2020-02-19 11:29:00	1.40	MAL1205435	1.40	MicroCal PEAQ-DSC...

MICROCAL PEAQ DASHBOARDS

LINK contains an extensive built-in dashboard library from LINK version 2.4.0.210401 and later. This function contains specific pre-created dashboards for all instruments and application groups.

CONTACT LUMETICS

For direct assistance, please contact Lumetics LINK™ Support:
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