

Chirascan – Applied Photophysics

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.

Chirascan is a CD system for analyzing biomolecules of all types and sizes. Chirascan data contributes to a deeper understanding of biomolecular characteristics, mechanisms, and interactions. More than α -helix and β sheet but determining the structural and thermodynamic properties of molecules.

DETAILS

LINK requires a CSV file to import Chirascan data. The following raw curve data will be imported, in addition to all available instrument/analysis settings and parameters calculated by the instrument software:

- Wavelength vs. Voltage
- Wavelength vs. Temp.
- Wavelength vs. HT
- Wavelength vs. Count
- Wavelength vs. CD

Notes:

- If there are files ending with the below, they will also be imported into the LINK software:
 - <root file name>p_Average.csv
 - <root file name>p_Baseline Subtracted.csv
 - <root file name>p_Standard Deviation.csv
- The process ("<root file name>p.csv") and unprocessed (<root file name>.csv) may contain more than one run, ie. replicates. LINK imports replicates as distinct measurements, except in the Baseline Subtracted case. These replicates columns are all filled with 0's, therefore they are not imported.
- An example list of sample files that might be imported with a root file name of "F10_BW0o5" are:
 - F10_BW0o5p.csv (processed file, contains all metadata)
 - F10_BW0o5.csv (unprocessed file also contains metadata)
 - F10_BW0o5p_Average.csv (contains one column of averaged data from all replicates)
 - F10_BW0o5p_Standard Deviation.csv (contains one column of standard deviation data from all replicates)
 - F10_BW0o5p_Baseline Subtracted.csv (contains one column, average of all columns of the p file, but with baseline subtracted)
- Note: Singe LINK requires the "root" file to end with a p.csv, be aware of same names ending with a 'p'.

The Chirscan CSV file example is as follows:

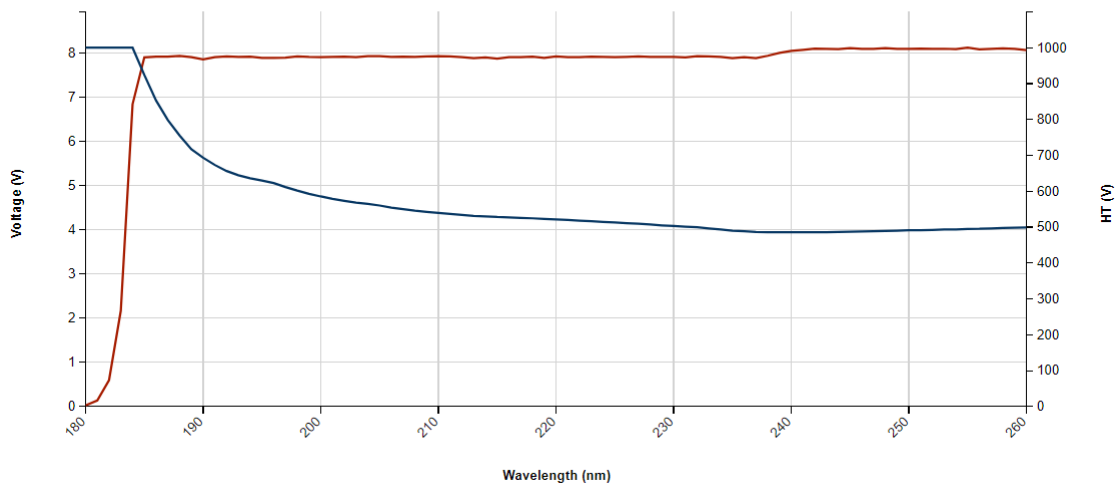
	A	B	C	D	E	F	G	H	I	J	K	
1	ProDataCSV											
2	Title: 2022_Sample_LINK											
3	Remarks:											
4	HV (CDDC channel)	438.812 v										
5	Time per point	1 s										
6	Description	Sample 1										
7	Concentration	0 M										
8	Pathlength	10										
9	Temperature	19.77 C										
10	Auto-Sampler Version	1.1.1585.82										
11	Cell Serial Number	2.5E+15										
12	Well ID	56										
13	Rack Name	rackone										
14	Well Label	Some Compound										
15	Sample Description	2022_LINK										
16	Current User	Chirscan User										
17	Chirscan-Auto Version	5.1.1585.82										
18	Emulated Chirscan	FALSE										
19	Validation Date	Monday April 10 2022 09:08:58										
20	Created	2022/09/05 15 10 40 (W. Europe Standard Time)										
21	Revision No 1 saved	2022/09/05 15 10 40 (W. Europe Standard Time)										
22	Is CFR Compliant	TRUE										
23	Is Raw	TRUE										
24	Available Dimensions:	2										
25	Wavelength	Wavelength Step Size: Bandwidth: 0.5nm										
26	Repeat	10 repeats -iter option selected										
27	Available Properties:	6										
28	Voltage											
29	Temperature											
30	HT											
31	Count											
32	CircularDichroism											
33	Absorbance											
34	Data:											
35	Voltage											
36	Wavelength	Repeat										
37		0	1	2	3	4	5	6	7	8	9	
38		260	8.04228	8.09508	8.00799	8.04259	8.06557	8.09127	8.03714	8.04023	8.09332	8.07921

EXAMPLES

Included below is a dashboard from Chirscan measurement files:

1. Line Chart plotting raw data curves for Voltage & HT vs. Wavelength

Voltage & HT vs. Wavelength



2. Tabular Summary examples

Measurement Summary Table – Measurement Results

Sample Name	Voltage (V) (Wavelength (nm) >1) - AVG	Temperature (°C) (Wavelength (nm) >1) - AVG	Particle Count (#) (Wavelength (nm) >1) - AVG	HT (V) (Wavelength (nm) >1) - AVG	CD (mdeg) (Wavelength (nm) >=2) - AVG	Count (Wavelength (nm) >=1) - AVG
Sample 1	614.27	1601.55	3240000.00	46717.49	-815.13	3240000.00
Sample 2	563.15	1467.99	2970000.00	42825.96	-866.07	2970000.00
Sample 3	497.35	1296.39	2622857.14	37821.27	-753.12	2622857.14
Sample 4	0.00	0.00	0.00	0.00	198.06	0.00

Measurement Summary Table – Instrument Settings

Sample Name	Validation Date	Concentration	Cell Serial Number - AVG	Analysis Date	Well ID - AVG	Repeat	Available Dimensions: - AVG
Sample 1	Monday, April 10, 20...	0 M	253002524147167...	Multiple (2 Values)	56	10 repeats in set., -it...	2
Sample 2	Monday, April 10, 20...	0 M	253002524147167...	Multiple (2 Values)	56	10 repeats in set., -it...	2
Sample 3	Monday, April 10, 20...	0 M	253002524147167...	Multiple (2 Values)	56	10 repeats in set., -it...	2
Sample 4	Monday, April 10, 20...	0 M	253002524147167...	2017-09-05 15:10:40	56	10 repeats in set., -it...	2

CHIRASCAN 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:

E-mail: support@lumetics.com

Phone: 1.613.417.1839

Website: <http://lumetics.com/>

