AuPRO – Pion

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.

AuPRO is a comprehensive data collection and refinement software. It provides the ability to analyze kinetic solubility and dissolution data. LINK address significant time savings for manipulating and overlaying AuPRO exported data.

DETAILS

LINK requires a user generated XLSX or XLSM file named "Study Design" to be present, and the associated AuPRO XLSX raw data file(s). The Study Design file must include a tab named "Combined Table" and/or "Sheet1" where critical experiment metadata field names on the first row, and the associated field values for Channels 1-6 on subsequent rows. The information withing the Study Design will inform LINK of the name of the AuPRO XLSX raw data file(s) present in the folder that should be imported, as well as provide information required for successful curve calculations. It may also provide information necessary to support advanced LINK functionality such as the ability to splice channel data together after a prescribed point in time from two separate AuPRO files.

Important AuPRO Information:
- The Study Design connects to the corresponding AuPRO XLSX data export via the Study Design "combined table" sheet fields; Vessel#/CH#, method.Filename Stage 1 and method.Filename Stage 2 (if applicable).
- The Study Design XLSX or XLSM and the AuPRO SLSX data export need to be in the same folder in order to be connected and imported into LINK.
- Within LINK, a field called "Measurement Type" will automatically be created, populated, and added to the Analysis Template Filter Panel to denote the curve types as Dissolution, Spectra or neither.
- A unique measurements/LINK Record ID is based on the following criteria: Analysis Date, File Name (study Design), Channel, Elapsed Time (min), Measurement Type, and Time Stamp.

The Study Design XLSX or XLSM has mandatory fields that must be present for successful import. These fields are located in the "Combined Table"/"Sheet1" tabs for importing Data from a specified 'Stage 1' AuPRO XLSX data file:

- Vessel#/CH#
- Total Dose per vessel (mg)
- method.Filename Stage 1
- method.Volume before Transfer (mL)

The Study Design XLSX or XLSM has mandatory fields that must be present for successful import for a channel splicing. These fields are located in the "Combined Table"/ "Sheet1" tabs for importing Data from a specified 'Stage 1' and 'Stage 2' AuPRO XLSX data files:

- Vessel#/CH#
- Total Dose per vessel (mg)
- method.Filename Stage 1
- method.Filename Stage 2
- method.Volume before Transfer (mL)
- method.Volume after Transfer (mL)
- method.Time for Transfer (min)
- method.Value before Transfer
- method.Value after Transfer

Upon import, LINK will perform calculate or import following curves:

- Concentration (µg/ml) vs. Time Stamp
- Concentration (µg/ml) vs. Elapsed Time
- AUC vs. Time Stamp
- AUC vs. Elapsed Time (min)
- % Drug Release vs. Time Stamp
- % Drug Release vs. Elapsed Time (min)
- CH Spectra: Absorbance (AU) vs. Wavelength (nm)
- STD Spectra: Absorbance (AU) vs. Wavelength (nm)

LINK calculates concentrations according to these formulas:

- Dosing Concentration Stage 1 (ug/ml): Total Dose per vessel (mg) * 1000 / method.Volume before Transfer (mL)
- Dosing Concentration Stage 2 (ug/ml): Total Dose per vessel (mg) * 1000 / method.Total Volume after transfer (mL)

The AuPRO XLSM file example is as follows:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1		CH1			CH2			CH3			CH4			CH5			CH6	
2	Min	µg/mL	AU	Min	µg/mL	AU	Min	µg/mL	AU	Min	µg/mL	AU	Min	µg/mL	AU	Min	µg/mL	AU
3	0.00	62.783730	0.0029	0.00	-5.431788	0.0008	0.00	-5.849417	0.0012	0.00	23.978071	0.0565	0.17	503.874115	0.0004	0.00	803.882263	0.0006
4	85.83	73.659775	0.1502	125.85	70.450897	0.1310	15.85	72.937027	0.1481	0.08	23.792376	0.0562	0.27	325.276184	0.0003	0.08	217.731644	0.0003
5	95.83	73.784027	0.1504	140.85	70.608376	0.1313	20.85	81.432808	0.1640	0.17	22.140997	0.0531	0.35	161.197403	0.0002	0.17	503.874115	0.0004
6	105.85	73.976334	0.1508	155.85	70.810356	0.1316	25.85	75.392220	0.1527	0.25	19.227383	0.0477	0.43	244.321442	0.0003	0.27	325.276184	0.0003
7	115.85	74.116684	0.1510	170.85	70.968750	0.1319	35.85	83.740433	0.1683	0.33	18.635687	0.0465	0.52	197.213318	0.0003	0.35	161.197403	0.0002

STD1 CH1   STD1 CH2   STD1 CH3   STD1 CH4   STD1 CH5   STD1 CH6   CH1   CH2   CH3   CH4   CH5   CH6   **Concentration1**   Stirrer Data   General Info   +

The AuPRO Study Design file example is as follows:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Vessel #/CH#	Unique Number/Formulation ID	Unique Method ID	Total Dose per vessel (mg)	Probe Path Length (mm)	Wavelength Selected (nm)	End of experiment pH	method. Method	method.Filename Stage	method.Filename Stage	method.Vessel Type	method.Stirring Mechanism	method.Time for Transfer (min)	method.Volume before Transfer (mL)
2	1	1	1	65	2 mm	250-258	5.5	2 Stage	LINK_Testing_Stage1	LINK_Testing_Stage2	LINK Vessels	Paddle	50	250
3	2	1	1	65	2 mm	250-258	5.5	3 Stage	LINK_Testing_Stage1	LINK_Testing_Stage2	LINK Vessels	Paddle	50	250
4	3	1	1	65	2 mm	250-258	5.5	4 Stage	LINK_Testing_Stage1	LINK_Testing_Stage2	LINK Vessels	Paddle	50	250
5	4	1	1	65	2 mm	250-258	5.5	5 Stage	LINK_Testing_Stage1	LINK_Testing_Stage2	LINK Vessels	Paddle	50	250
6	5	1	1	65	2 mm	250-258	5.5	5 Stage	LINK_Testing_Stage1	LINK_Testing_Stage2	LINK Vessels	Paddle	50	
7														

General Information   Formulation Sample Details   Method   Study Design   Lists   **Combined Table**   Common Media List Cheat list   +

The AuPRO-specific import method options are available for all AuPRO import types. The import method default settings are:

- Curve Import Options: Default does not include CH Spectra or STD CH Spectra
- Study Design: Default is to not include the study design as an attachment.
- Automated metadata extraction: None

The AuPRO-specific import method setting includes Curve Import Options. This option allows the import of spectrum data found in the 'CH 1-8' tabs or spectra or 'STD1 CH1-8' tabs if present in the XLXS workbook. By default, LINK will not import the spectra.

Curve Import Options

AuPro: Select to import the spectrum data found in the 'CH1-8' tabs, or spectra or 'STD1 CH1-8' tabs found in the XLSX workbook (if present).

☐ Include CH Spectra

☐ Include STD CH Spectra

Default value is to not import the CH or STD CH spectra data.

Cancel   Back   Next

The AuPRO-specific import method setting includes the ability to save the Study Design XLSX/XLSM file as an attachment to the imported measurements(s).

Study Design

Select the checkbox below to include the Study Design XLSX/XLSM file as an attachment to the imported measurements(s).

☐ Include Study Design XLSX/XLSM file as Attachment.

| Cancel | Back | Next |

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.
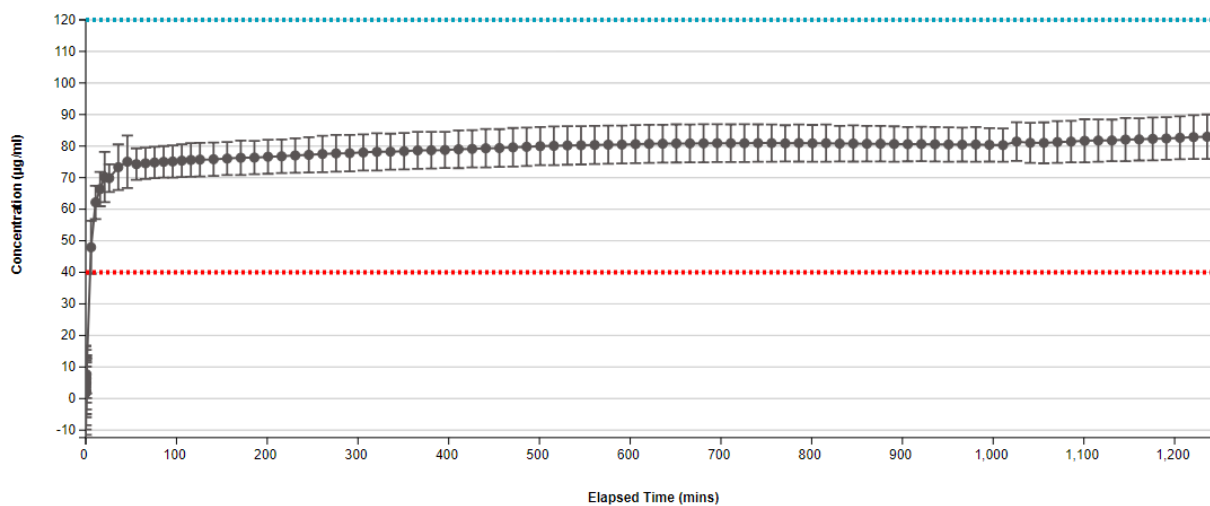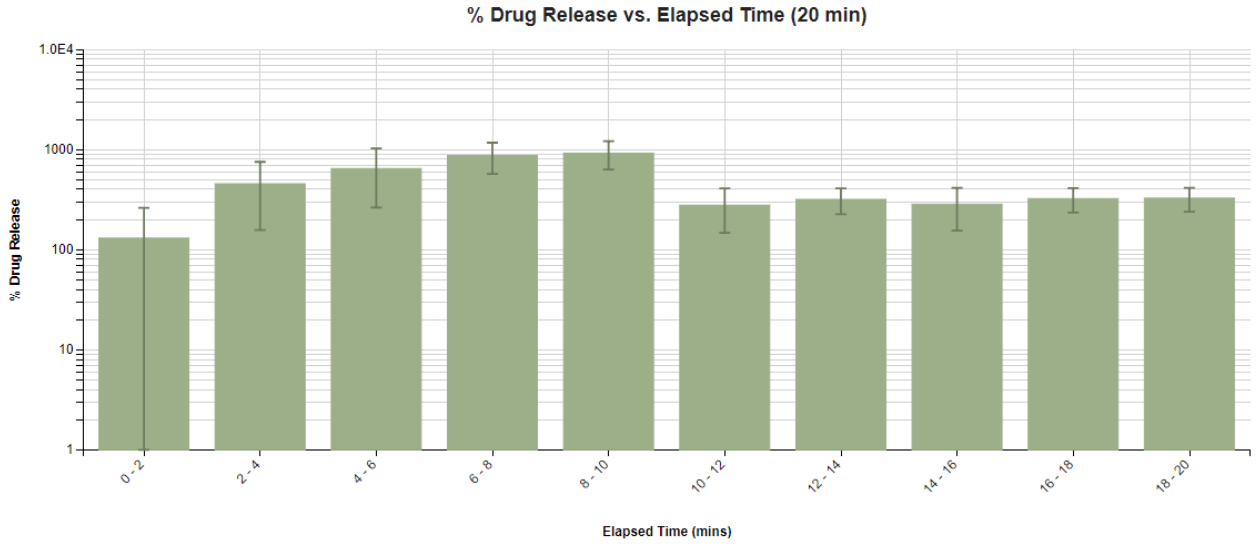
EXAMPLES

Included below are example dashboards from AuPRO measurement files:

1. Line Chart plotting raw data curves for Concentration vs. Elapsed Time

Concentration vs. Time

2. Histogram plotting %Drug release vs. Elapsed time in 2-minute bin intervals to 20 minutes

% Drug Release vs. Elapsed Time (20 min)

3. Chart stats table configured to represent the above %Drug Release histogram chart

						AuPRO, Total Population, % Drug Release				
Elapsed Time (mins)	Bin Center	Measurements	Mean	Stdev	MIN	MAX	RSD	SE	Lower 95% CI	Upper 95% CI
0 - 2	1.00	33	130.32	131.23	-11.72	523.89	1.01	22.84	85.55	175.09
2 - 4	3.00	29	454.52	297.61	0.11	1,182.90	0.65	55.26	346.21	562.84
4 - 6	5.00	33	645.53	382.35	12.38	1,223.55	0.59	66.56	515.08	775.98
6 - 8	7.00	29	869.89	299.64	127.96	1,229.66	0.34	55.64	760.83	978.95
8 - 10	9.00	29	920.03	289.33	146.71	1,258.26	0.31	53.73	814.73	1,025.34
10 - 12	11.00	33	277.87	130.92	18.32	425.71	0.47	22.79	233.20	322.54
12 - 14	13.00	29	317.46	91.96	57.31	428.31	0.29	17.08	283.99	350.92
14 - 16	15.00	33	284.38	129.88	19.88	431.13	0.46	22.61	240.07	328.69
16 - 18	17.00	29	323.61	88.63	63.63	433.89	0.27	16.46	291.36	355.87
18 - 20	19.00	29	326.89	87.39	65.35	438.39	0.27	16.23	295.08	358.69

4. Tabular Summary examples

Measurement Summary Table – Instrument Settings

Title	Sample Name	Aupro Version	method.Stirring RPM - AVG	method.Temperature (DegC)	method.Stirring Mechanism	method.Probe	Baseline correction method
Evaluation of LINK Testing Examples	Sample A	6	75	37	Paddle	L Shape	Second Derivative
Evaluation of LINK Testing Examples	Sample B	6	75	37	Paddle	L Shape	Second Derivative
Evaluation of LINK Testing Examples	Sample C	6	75	37	Paddle	L Shape	Second Derivative
Evaluation of LINK Testing Examples	Sample D	6	75	37	Paddle	L Shape	Second Derivative
Evaluation of LINK Testing Examples	Sample E	6	75	37	Paddle	L Shape	Second Derivative
Evaluation of LINK Testing Examples	Sample F	6	75	37	Paddle	L Shape	Second Derivative

Measurement Summary Table – Experiment Design

Vessel #/CH#	method.Method	Unique Method ID	Unique Number/ Formulat ion ID	LNK_Import_ Data_Splicing	method.Time for Transfer (min)	method.Volume before Transfer (mL)	method.Volume added for transfer (mL)	method.Total Volume after transfer (mL)	Total Dose per vessel (mg)	Dosing Concentration Stage 1 (ug/ml)	Dosing Concentration Stage 2 (ug/ml)	method .Vessel Type	End of experiment pH	method. Media for transfer	method.Media after the transfer
1	2 stage	1	1	Yes	15	250	550	650	2.50	8	2	LINK vessels	6.50	pH 7.1	buffer pH 7
2	2 stage	1	1	Yes	15	250	550	650	2.50	8	2	LINK vessels	6.50	pH 7.1	buffer pH 7
3	2 stage	1	1	Yes	15	250	550	650	2.50	8	2	LINK vessels	6.50	pH 7.1	buffer pH 7
4	2 stage	2	1	Yes	15	250	550	650	2.50	8	2	LINK vessels	6.50	pH 7.1	buffer pH 7
5	2 stage	2	1	Yes	15	250	550	650	2.50	8	2	LINK vessels	6.50	pH 7.1	buffer pH 7

CONTACT LUMETICS

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