OpenLAB/ ChemStation – Agilent

Compatible with LC, GC, CE, CE/MS, and LC/MS instruments systems

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.

OpenLAB/ChemStation is software compatible with Agilent LC, GC, CE, CE/MS, and LC/MS instruments systems. Method Scouting Wizard creates a sample sequence containing all possible combinations of available columns, solvents, a set of predefined gradients and a set of predefined temperatures.

DETAILS

LINK requires a TXT data file exported from the OpenLAB software. A valid TXT file must start with 'Data File' or be in a table format stating with 'SEC Report with Detail'. A CSV export of the chromatogram data is optional and if a PDF instrument report is present, it needs to have the exact same name as the TXT report to be imported to LINK and be available as a Measurement Series Attachment. All other files including acq.text, intermediate.txt and rpthead.txt are skipped.

Helpful Notes:

- The CSV file(s) *must* be named the same as the signal name (e.g., ***dad1a.csv***, case-insensitive).
- If the TXT report file contains a signal table with no peaks found, this signal/measurement will not be imported at all.
- Unique measurements are fined by unique values for: SampleName, Single/Channel, AnalysisDate

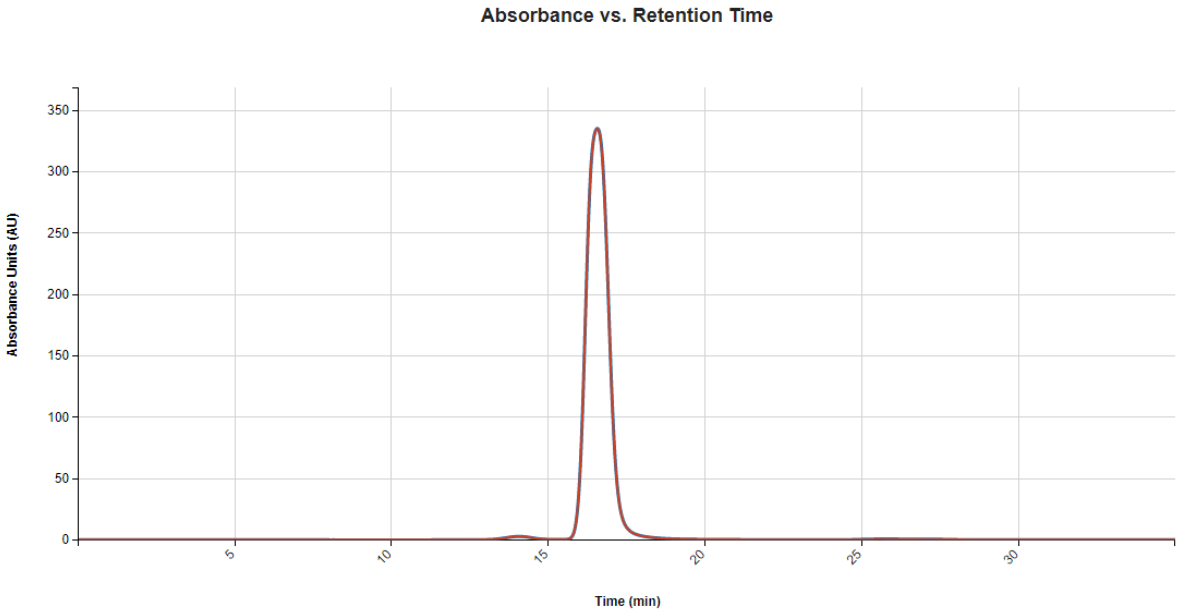
The ChemStation TXT data file example is as follows:

```
Data File C:\Chem32\1\Data\
Sample Name: Sample A
HDR HPLC 11/3/2017 4:38:38 PM SYSTEM

=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
Acq. Instrument : HDR HPLC                      Location :   1
Injection Date  : 11/3/2017 4:03:36 PM               Inj :   1
                                               Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 20.000 µl
Sequence File   : C:\Chem32
Method          : C:\Chem32
Last changed    : 11/3/2017 4:02:43 PM by SYSTEM
Method Info     : SEC method:
                  Mobile phase:
                  40mM Na-Phosphate, 150mM NaCl, pH 7.2.
                  column: TSk gel G3000SWxl ( p/n 08541, Column # 08B-02386B)
                  Guard column TSK gel Guard SWxL colum (p/n 08543, Column no 90B-01508B)
                  Flow 0.45ml/min, time 35 min
                  Monitor at 280nm

=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 G, Sig=280,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.667 BB    0.6960 1.64743e4   382.88959  99.6039
   2  25.667 BB    0.2124   65.51289    4.59192   0.3961
Totals :                 1.65398e4   387.48150
```

EXAMPLES

Included below is a sample dashboard from OpenLAB/ChemStation measurement files:

1. Line Chart plotting raw data curves for Absorbance vs. Time



2. Tabular Summary examples

Measurement Summary Table – Measurement Results

LINK Record ID #	Peak Count - AVG	Absorbance (AU) (Retention Time (min) >=1) - AVG	Absorbance (AU) (Time (min) <1) - AVG	Peak 1 Area (%) - AVG	Max Peak Width (min) - AVG	Max Peak Type	Max Peak RetTime (min) - AVG	Max Peak Height (mAU) - AVG	Max Peak Area (%) - AVG
1	1	0.00	0.00	100.00	0.75	BBA	16.43	302.26	100.00
2	4	0.00	0.00	0.98	0.76	BB	16.41	1734.26	98.88
3	1	0.00	0.00	100.00	0.79	BB	16.43	109.91	100.00
4	1	0.00	0.00	100.00	0.75	BBA	16.44	312.56	100.00
5	3	0.00	0.00	1.21	0.76	VB	16.42	1795.91	98.56
6	1	0.00	0.00	100.00	0.79	BB	16.44	113.81	100.00
7	1	0.00	0.00	100.00	0.75	BBA	16.43	340.56	100.00
8	3	0.00	0.00	0.94	0.76	BB	16.41	1946.15	99.02
9	1	0.00	0.00	100.00	0.78	BB	16.43	123.82	100.00
10	1	0.00	0.00	100.00	0.75	BBA	16.43	308.46	100.00

Measurement Summary Table – Instrument Settings

LINK Record ID #	File Name	Signal	Location	Seq. Line - AVG	Injection Date	Inj Volume	4 Ref - AVG
1	Report.TXT	DAD1 G	D2B-A1	59	11/8/2017 10:04:05 PM	5.000 µl	360
2	Report.TXT	LNG1 G	D2B-A1	59	11/8/2017 10:04:05 PM	5.000 µl	360
3	Report.TXT	SHT1 G	D2B-A1	59	11/8/2017 10:04:05 PM	5.000 µl	360
4	Report.TXT	DAD1 G	D2B-A2	60	11/8/2017 10:39:50 PM	5.000 µl	360
5	Report.TXT	LNG1 G	D2B-A2	60	11/8/2017 10:39:50 PM	5.000 µl	360
6	Report.TXT	SHT1 G	D2B-A2	60	11/8/2017 10:39:50 PM	5.000 µl	360
7	Report.TXT	DAD1 G	D2B-A3	61	11/8/2017 11:15:34 PM	5.000 µl	360
8	Report.TXT	LNG1 G	D2B-A3	61	11/8/2017 11:15:34 PM	5.000 µl	360
9	Report.TXT	SHT1 G	D2B-A3	61	11/8/2017 11:15:34 PM	5.000 µl	360
10	Report.TXT	DAD1 G	D2B-A4	62	11/8/2017 11:51:19 PM	5.000 µl	360

CHEMSTATION/OPENLAB 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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