

FT-IR Spectrometer – Bruker

ALPHA II, Invenio, HTS-XT

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.

Fourier-transform infrared spectroscopy (FTIR) is a technique used to obtain an infrared spectrum of absorption or emission of a solid, liquid or gas. An FTIR spectrometer simultaneously collects high-spectral-resolution data over a wide spectral range. Bruker FT-IR Spectrometers are intelligent systems for analytical and demanding R&D.

DETAILS

LINK requires JCAMP or dpt. file formats. The JCAMP file is generated automatically by the FT-IR software.

The Bruker JCAMP file example is as follows:

```
1  ##TITLE=26-Feb-2020_SampleDescription
2  ##JCAMP-DX=4.24
3  ##DATA TYPE=INFRARED SPECTRUM
4  ##DATE=26/2/2020
5  ##SAMPLING PROCEDURE=26-Feb-2020_SampleDescription_February_13_2020
6  ##ORIGIN=Kristie Somers
7  ##XUNITS=1/CM
8  ##YUNITS=ABSORBANCE
9  ##RESOLUTION=4
10 ##FIRSTX=3098.7622
11 ##LASTX=999.83107
12 ##DELTAX=-0.71416505
13 ##MAXY=0.0067420583
14 ##MINY=-0.052551929
15 ##XFACTOR=1
16 ##YFACTOR=4.8942798e-11
17 ##NPOINTS=2940
18 ##FIRSTY=-0.041195963
19 ##XYDATA=(X++(Y..Y))
20 3098.76-841716544-840535997-839333149-838041626-836607464-835014145-833290516
21 3093.76-831477072-829612097-827735249-825863729-823991828-822132105-820259443
22 3088.76-818396981-816557277-814742310-812975144-811249232-809569294-807922846
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```

The following raw curve data may be imported via dpt. file, in addition to all available instrument/analysis settings and parameters calculated by the instrument software:

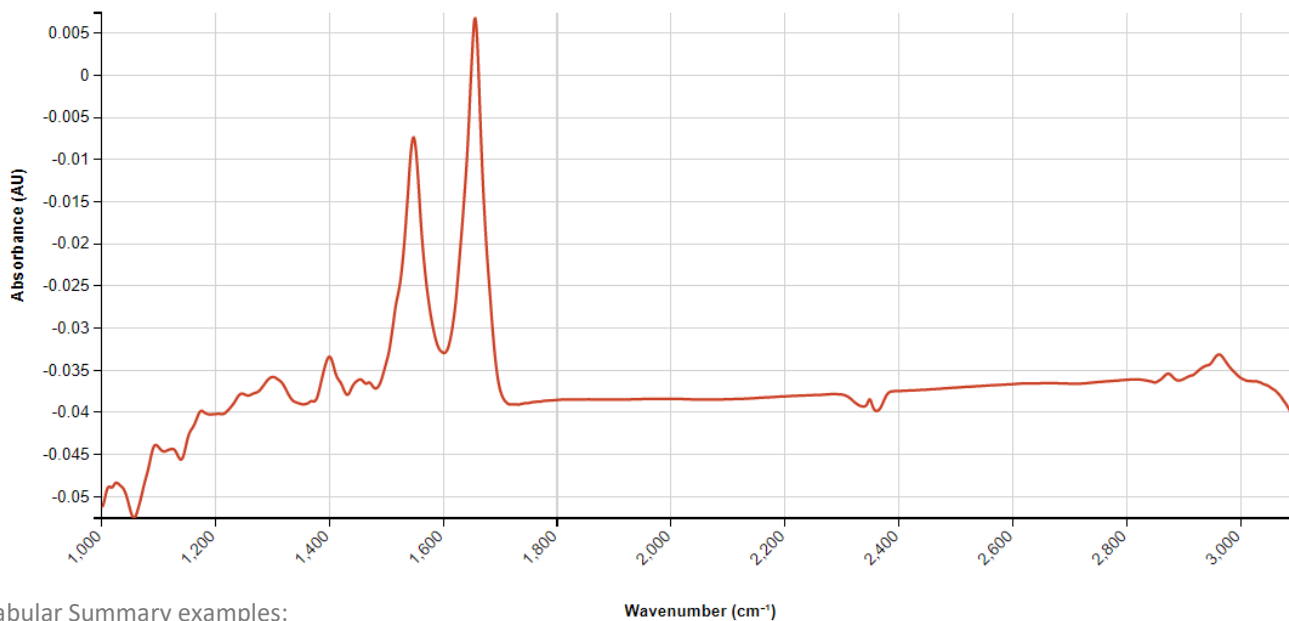
- Absorbance vs. Wavenumber (cm⁻¹)

EXAMPLES

Included below are sample dashboards from Bruker FT-IR measurement files:

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

Absorbance vs. Wavenumber



2. Tabular Summary examples:

Measurement Summary Table – Measurement Results

LINK Record ID #	Sample Name	Absorbance (AU) (Wavenumber (cm ⁻¹) >=5) - AVG	JCAMP-DX - AVG	RESOLUTION - AVG	MINY - AVG	MAXY - AVG	LASTX - AVG	FIRSTY - AVG	FIRSTX - AVG	DELTA - AVG
1	Sample A	-107.90	4.24	4	-0.05	0.01	999.83	-0.04	3098.76	-0.71
2	Sample B	-107.90	4.24	4	-0.05	0.01	999.83	-0.04	3098.76	-0.71

Measurement Summary Table – Instrument Settings

LINK Record ID #	Operator	Sample Name	File Name	Version	XFACTOR - AVG	YFACTOR - AVG	YUNITS	XUNITS	DATA TYPE
1	Lumetics 1	Sample A	27-Feb-2020_B...	JCAMP-DX4.24	1	0.00	ABSORBANCE	1/CM	INFRARED SPE...
2	Lumetics 2	Sample B	27feb2020-JCA...	JCAMP-DX4.24	1	0.00	ABSORBANCE	1/CM	INFRARED SPE...

BRUKER FT-IR 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

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