



Worldwide MIR Spectra Standardization

**Bentley IR Cell and Spectra standardization
A new highly effective and simple approach (patented)**

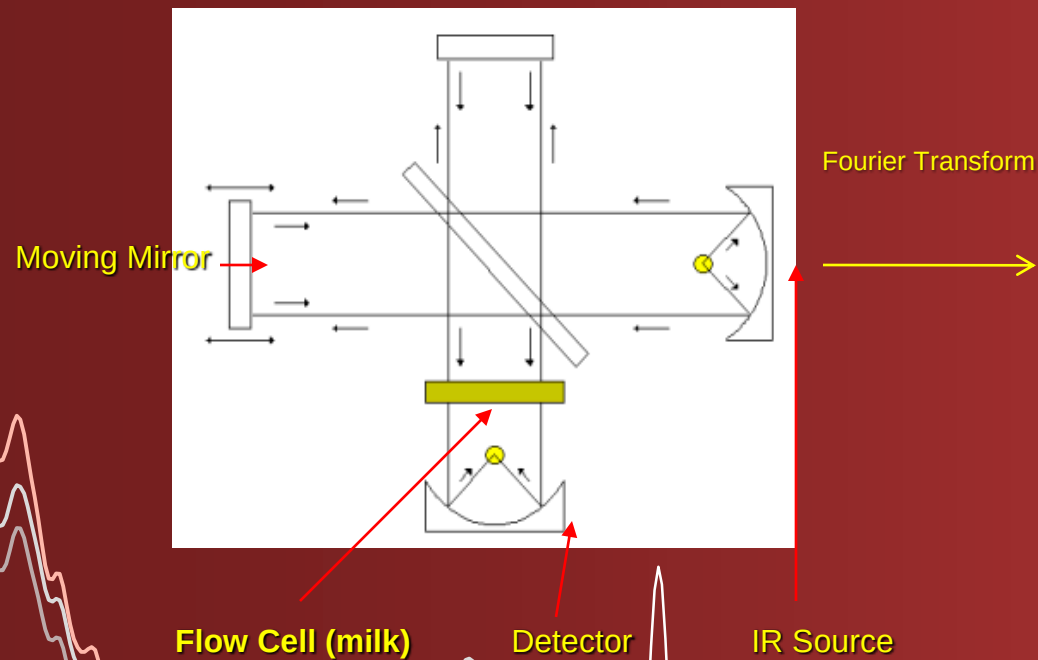
*By Pierre Broutin
Managing Director/Senior Scientist*



ICAR 2016 Congress Manufacturers Showcase, Puerto Varas, Chile
October 27, 2016

Bentley FTMIR Optical Deck

INTERFEROMETER



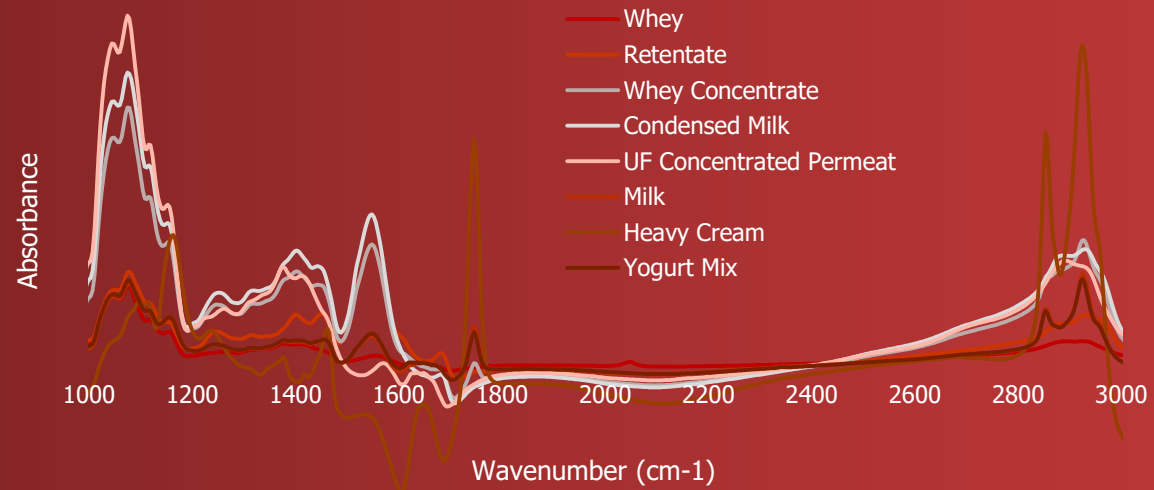
MILK SPECTRUM





Bentley FTS/DairySpec

Milk Components Absorption wavebands



Bentley IR Cell and Spectra standardization

Why?

- Interferometer laser frequency can vary over time ➡ spectrum x axis shift
- Flow cell pathlength can increase over time ➡ spectrum y axis shift

Thus, spectra standardization is very important:

- For optimum calibration transfer between instruments
- For worldwide equivalence of analytical results
- For results/calibration stability (Slope/Bias)
- To reduce calibration development cost (centralized calibrations)
- For implementation of qualitative spectral analysis





Bentley IR Cell and Spectra standardization

A new highly effective and simple approach

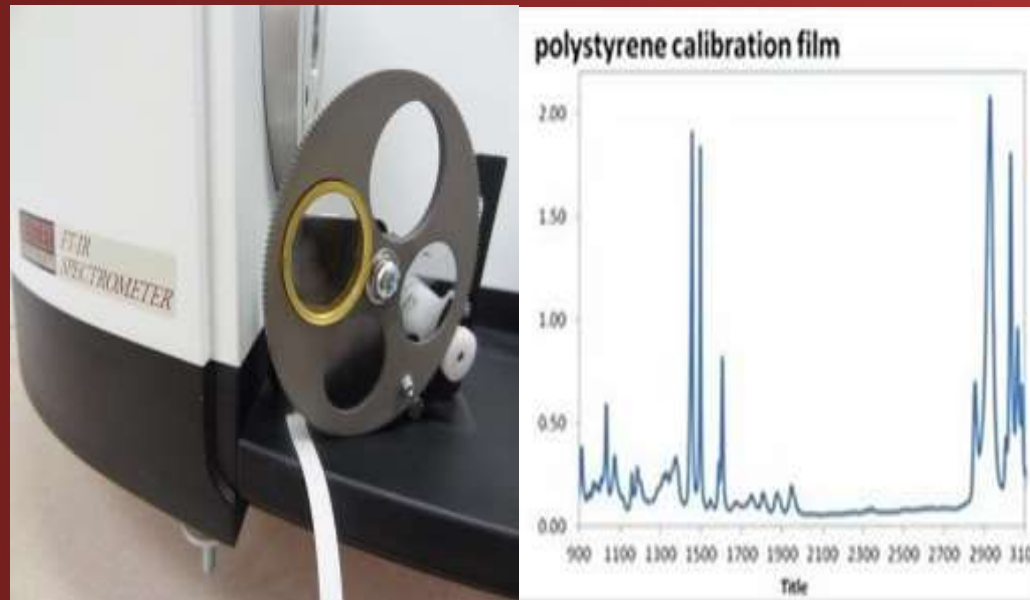
Prerequisites to standardize the infrared spectra:

- 1 - Standardization of spectrum x axis (wavenumbers)
- 2 - Standardization of spectrum y axis (absorbance)
- 3 - Standardization of all operating conditions and sample preparation
- 4 - Removal of any moisture in optical deck that could affect the spectra



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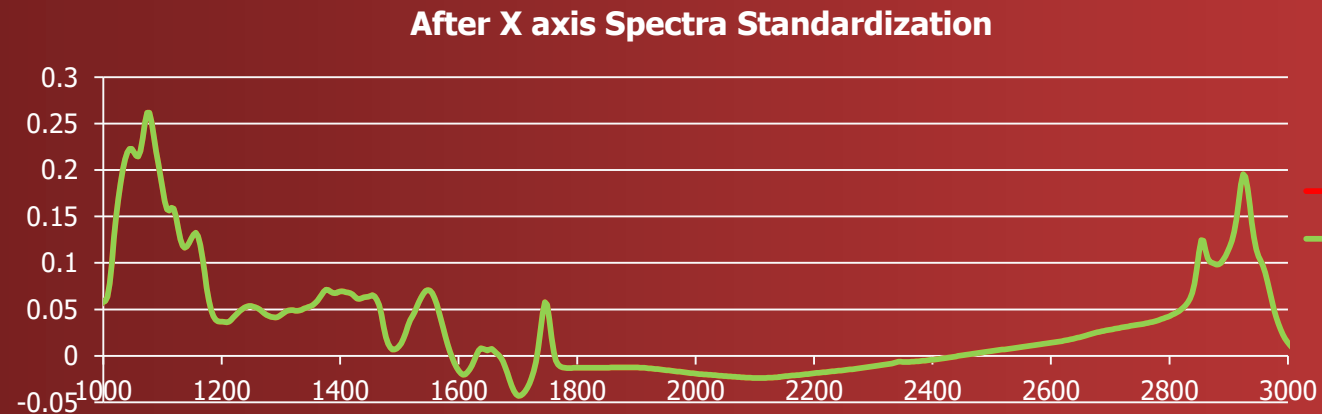
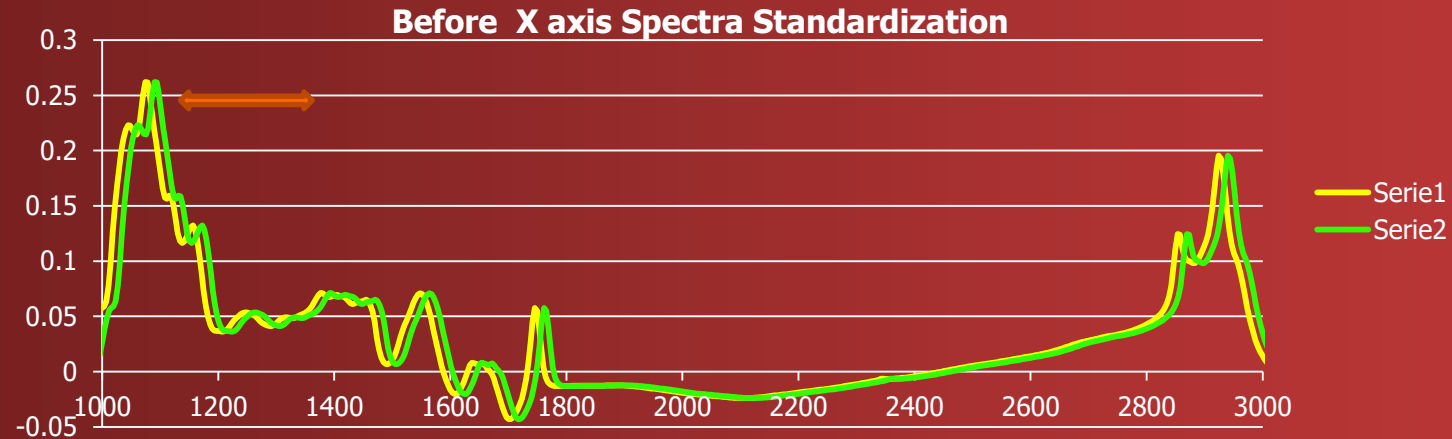
1 - Standardization of spectrum x axis with a polystyrene film (internationally recognized NIST standard) to calibrate optimally interferometer laser frequency



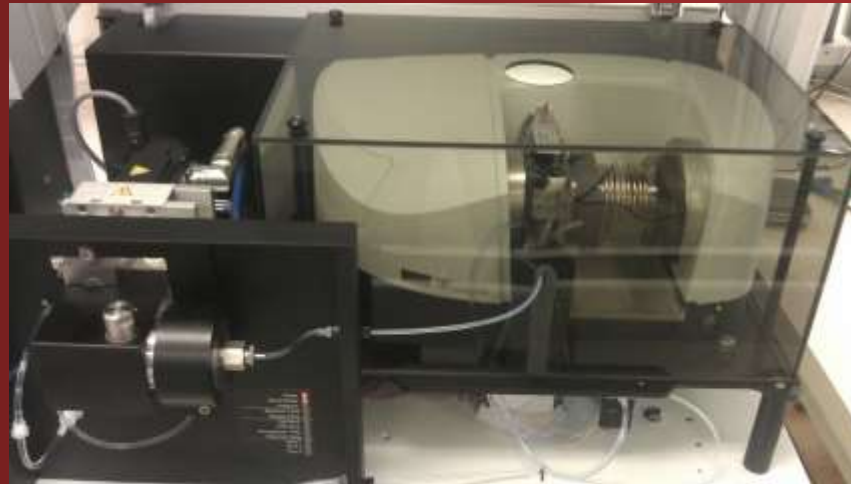
■Example: Polystyrene Test

- [4:30 PM Central Daylight Time] Polystyrene Test: STARTED
- Background Scan Completed
- Polystyrene Scan Completed
- Peak 3082.22 @:3082.18 cm-1
- Peak 3060.14 @:3060.12 cm-1
- Peak 1601.38 @:1601.37 cm-1
- Peak 1583.04 @:1583.24 cm-1
- Peak 1028.42 @:1028.59 cm-1
- [4:31 PM Central Daylight Time] Polystyrene Test: PASSED
-

**1 - Standardization of spectrum x axis with
a polystyrene film (internationally recognized NIST standard) to
calibrate optimally interferometer laser frequency**

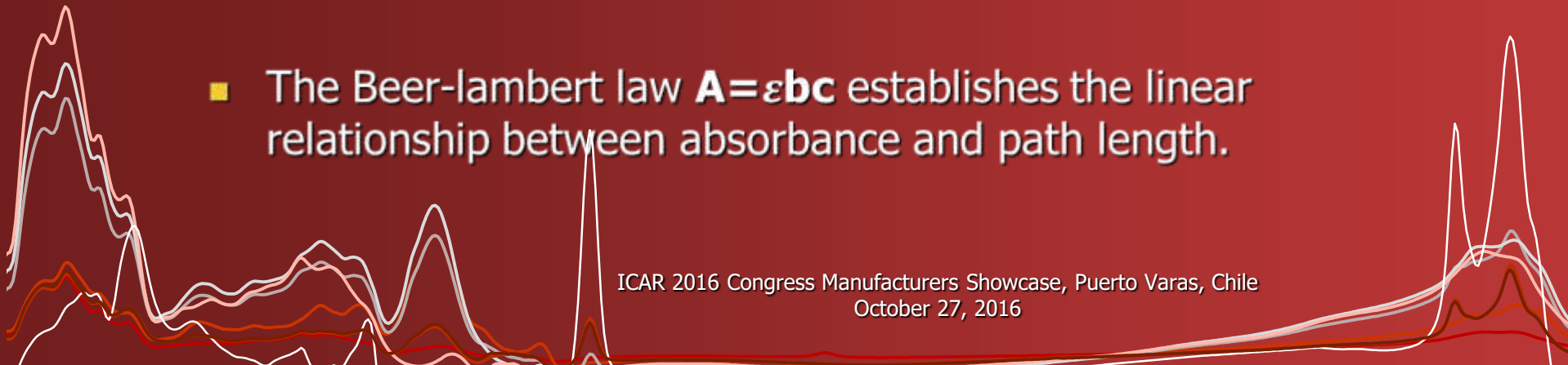


2 - Standardization of spectrum y axis (absorbance) by measuring very accurately and in real time the IR flow cell thickness(patented)

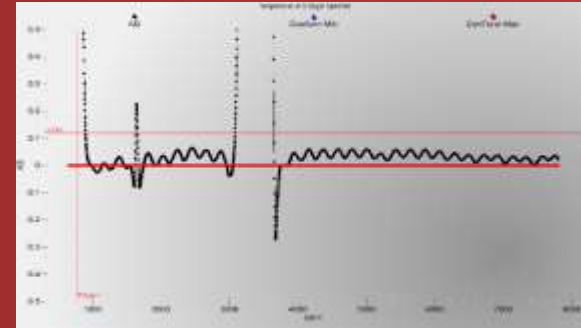
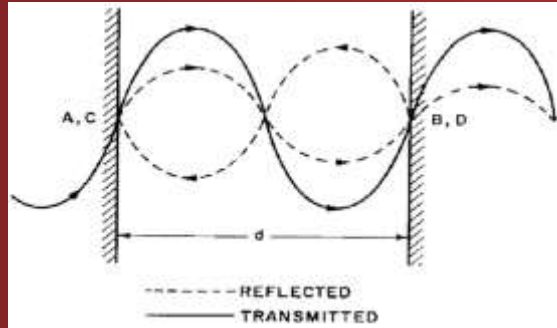


2 - Standardization of spectrum y axis (absorbance) by measuring very accurately and in real time the IR flow cell thickness (patented)

- The thickness of the sealed cells is one of the basic measurements required for quantitative analysis.
- The cell thickness should be verified from time to time frequency depending on the type of products analyzed, since it may change due to a gradual erosion of the cell internal surfaces (1% per month, up to 12% per year).
- The Beer-lambert law **$A = \epsilon bc$** establishes the linear relationship between absorbance and path length.



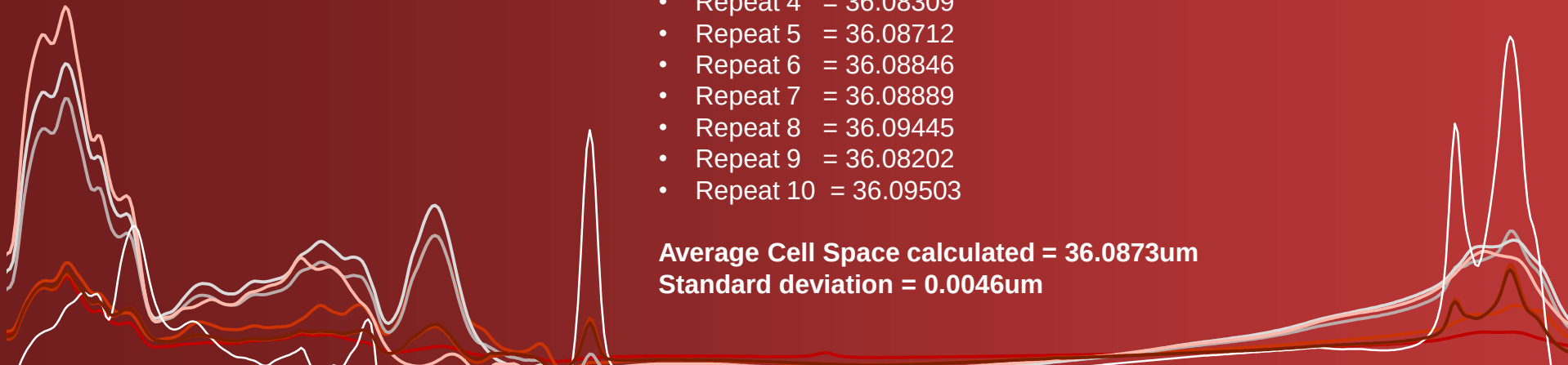
2 - Standardization of spectrum y axis (absorbance) by measuring very accurately and in real time the IR flow cell thickness (patented)



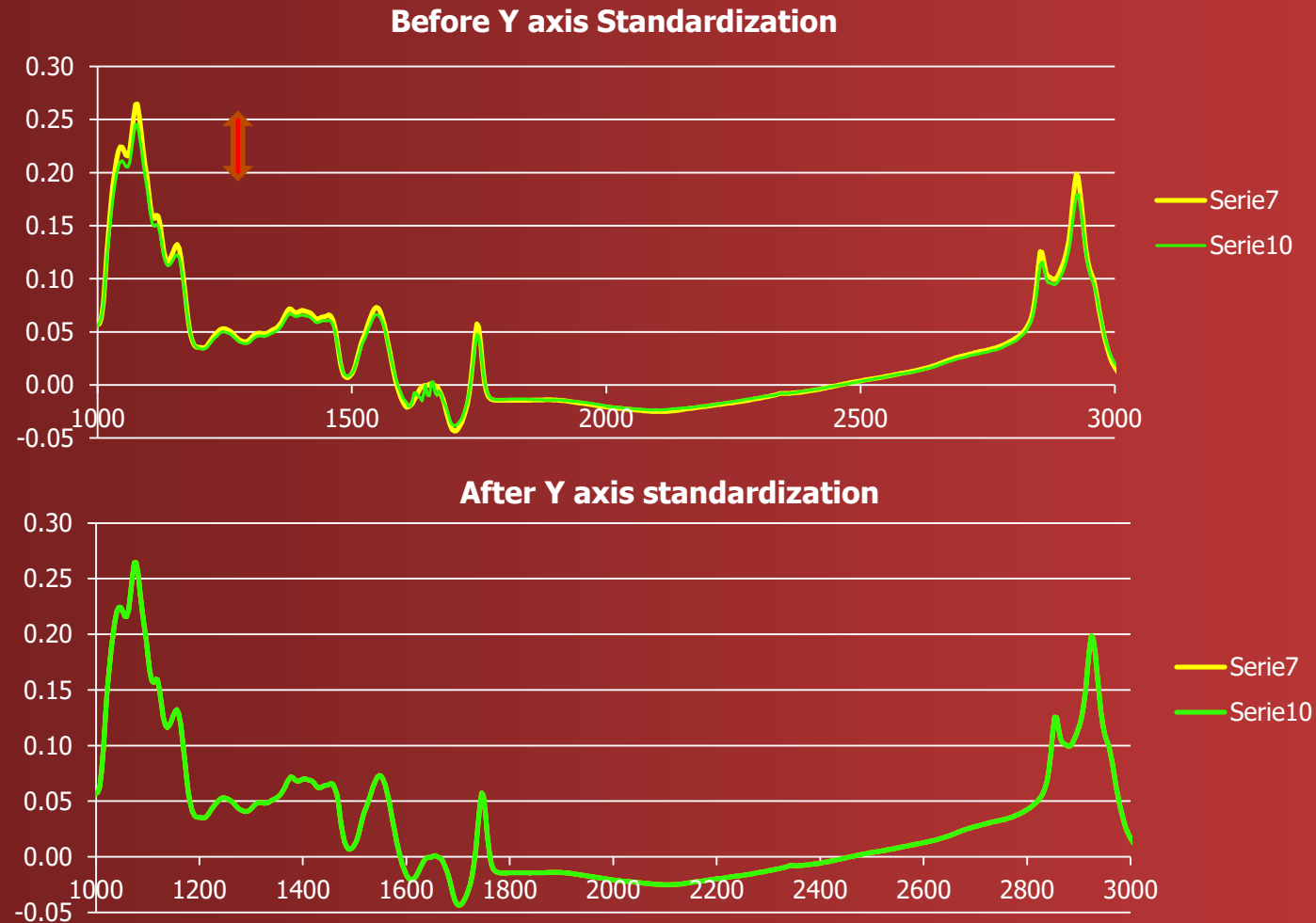
Summary Report

- Repeat 1 = 36.08468
- Repeat 2 = 36.08663
- Repeat 3 = 36.08227
- Repeat 4 = 36.08309
- Repeat 5 = 36.08712
- Repeat 6 = 36.08846
- Repeat 7 = 36.08889
- Repeat 8 = 36.09445
- Repeat 9 = 36.08202
- Repeat 10 = 36.09503

Average Cell Space calculated = 36.0873um
Standard deviation = 0.0046um



2 - Standardization of spectrum y axis (absorbance) by measuring very accurately and in real time the IR flow cell thickness (patented)



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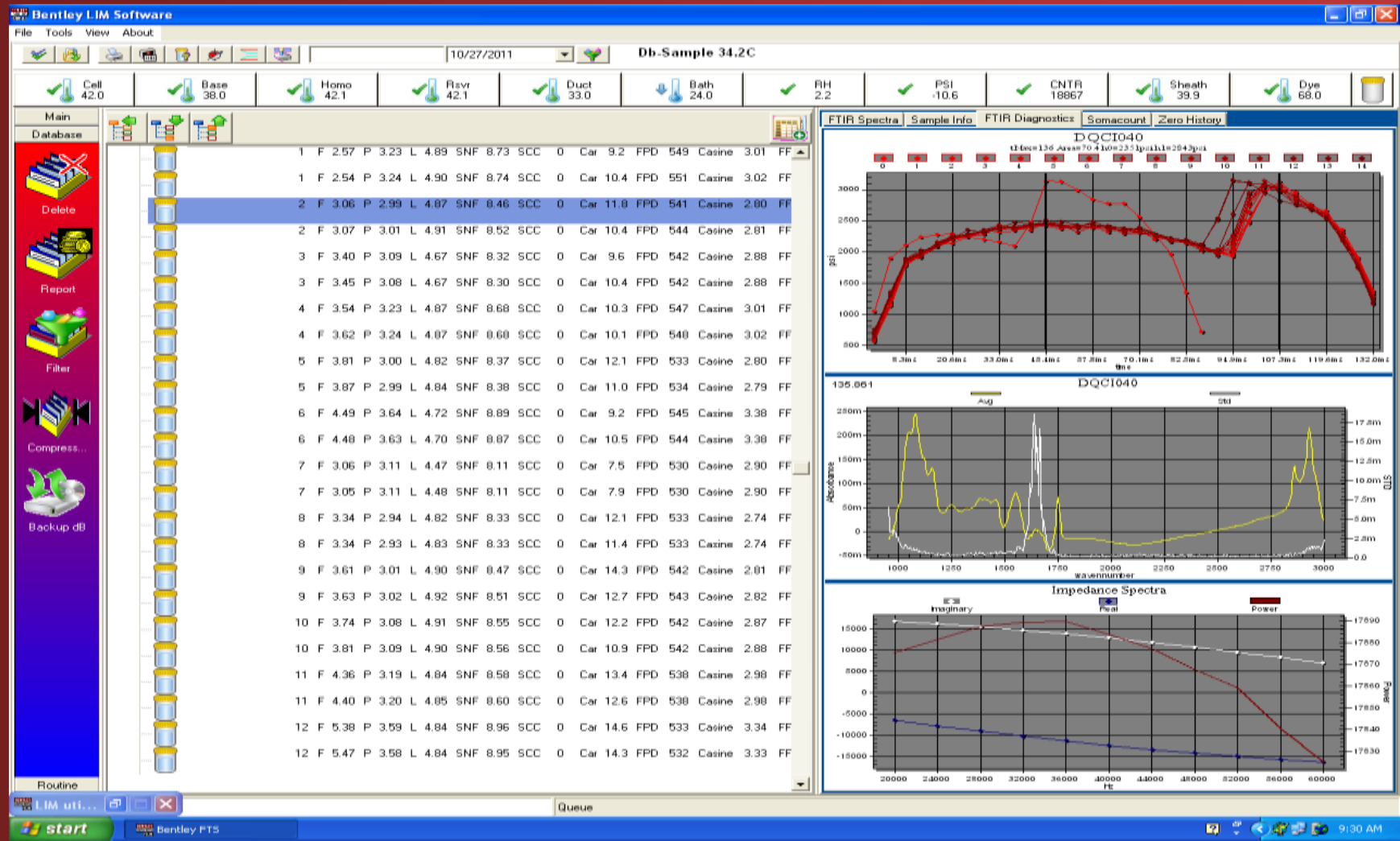
Why this way?

- Laser calibrated with NIST traceable films (polystyrene)
- Does not require any highly accurate liquid mixtures
- No consumable to package, store, maintain or process
- Automatic execution, no user dependent operations
- Can be performed as often as necessary
- **A very reliable, easy to implement, and cost effective solution**



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3 - Standardization of all operating conditions and sample preparation



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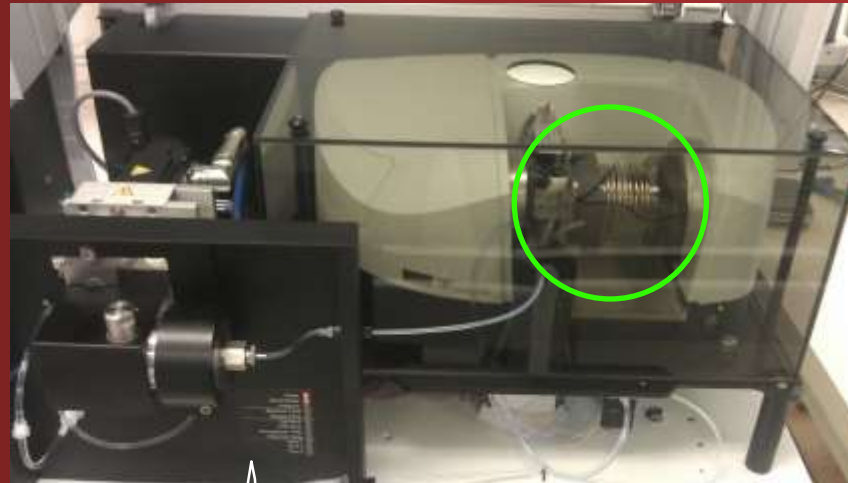
Full standardization of all operating conditions:

- Samples mixing/shaking
- Sample temperature
- Sample heating time

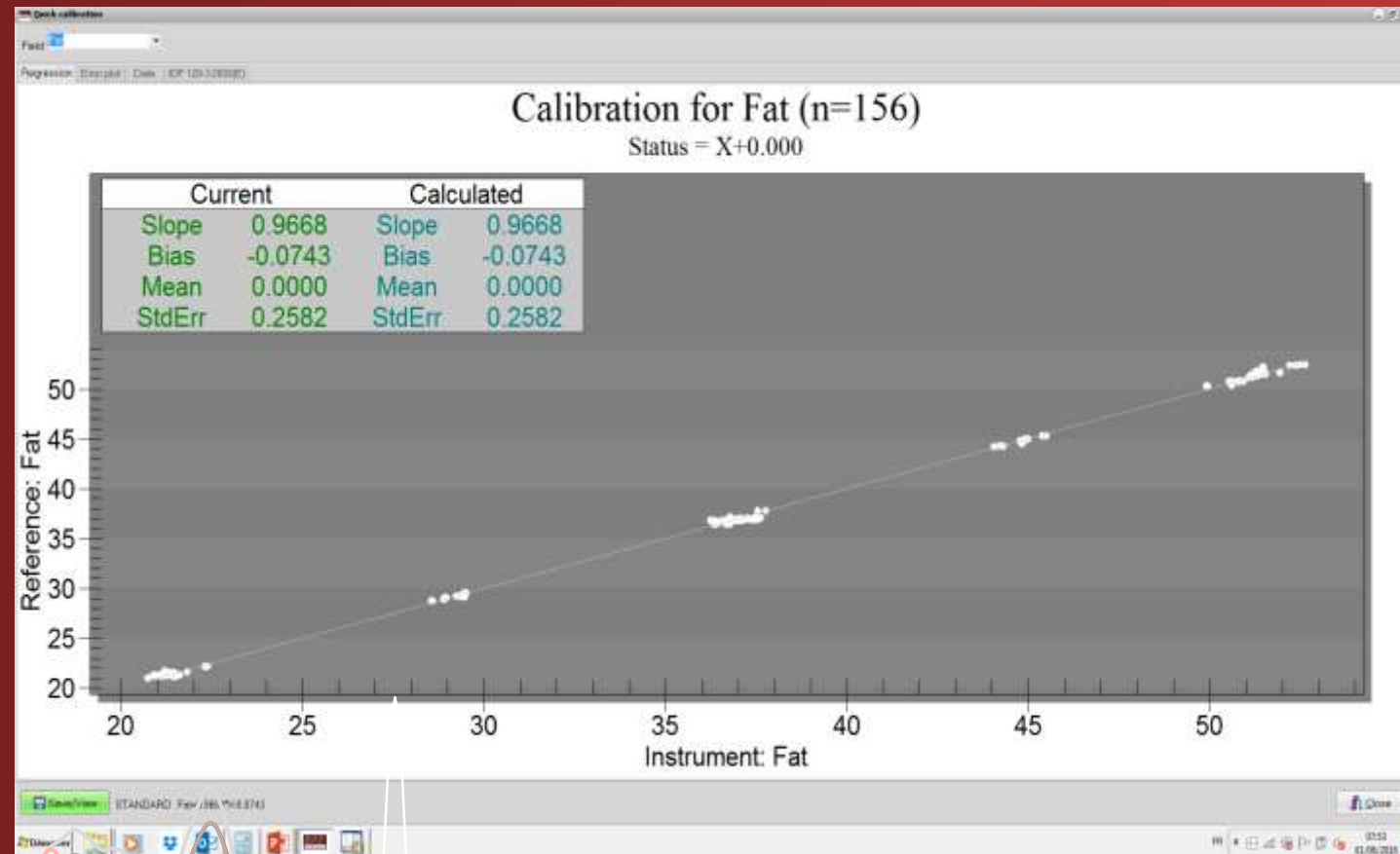
Samples handling independent of operators and highly reproducible

4 - Removal of any moisture in optical deck that interfere with spectra

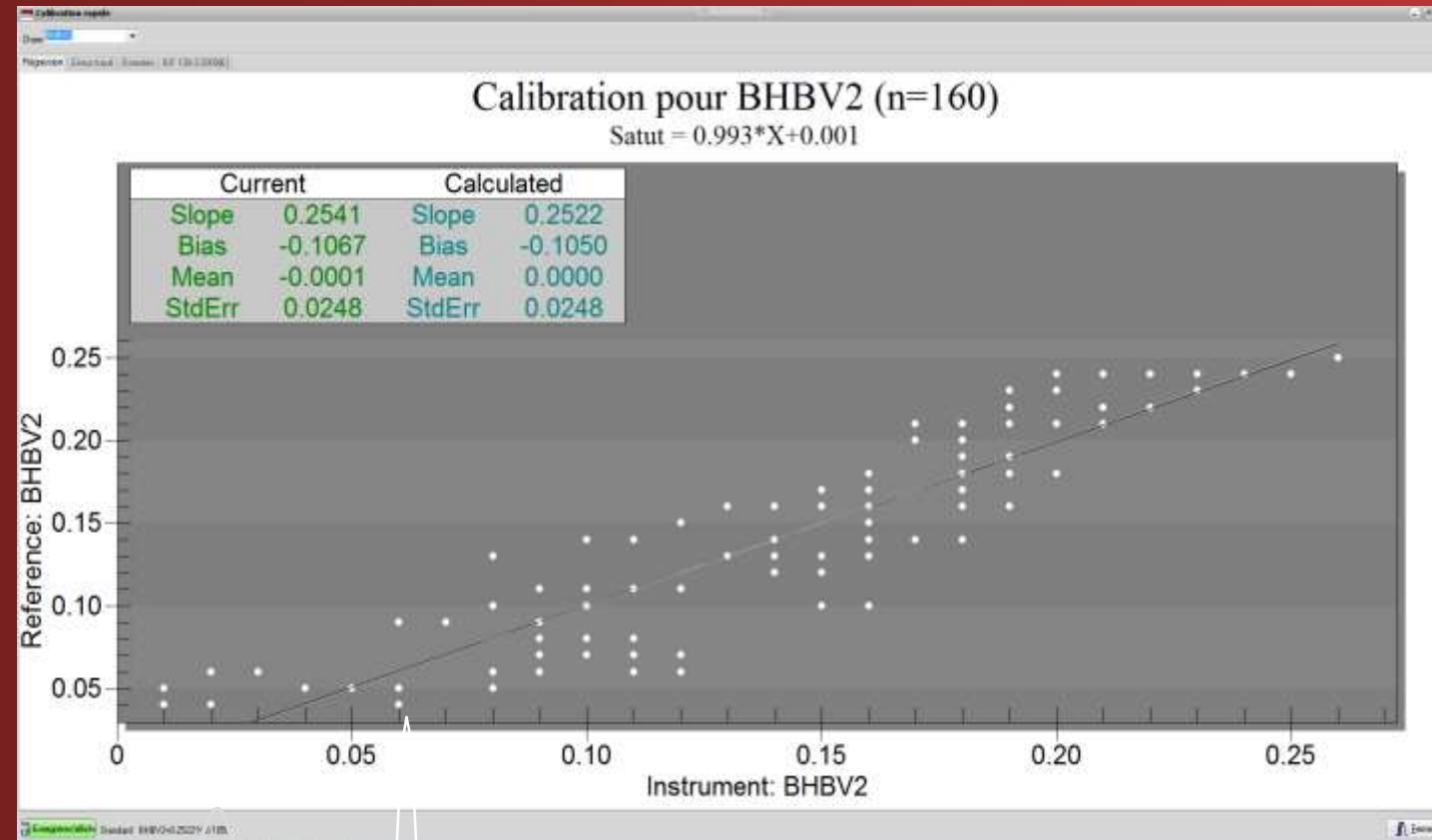
- The optical deck sealed to remove all potential interference
- The cell isolated outside the optical deck in a small elbow containing a dessicant
- The optical deck moisture level is also monitored in real time.

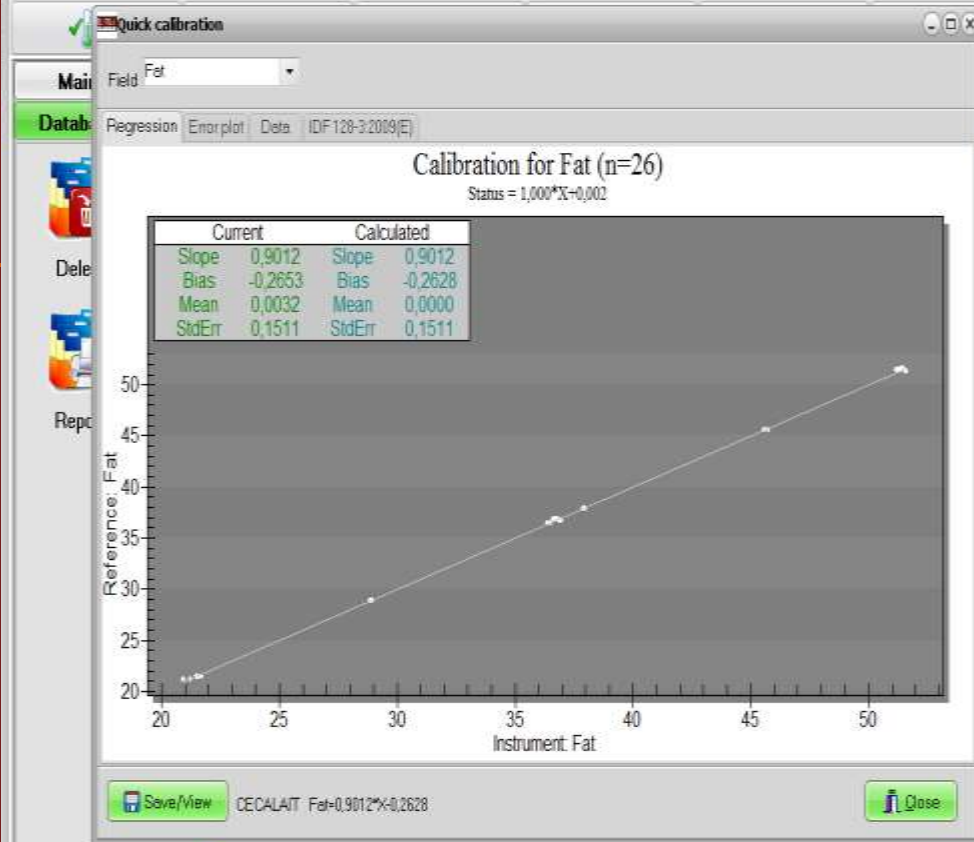


CECALAIT Calibration samples analyzed over 7 months – single calibration, no adjustment required

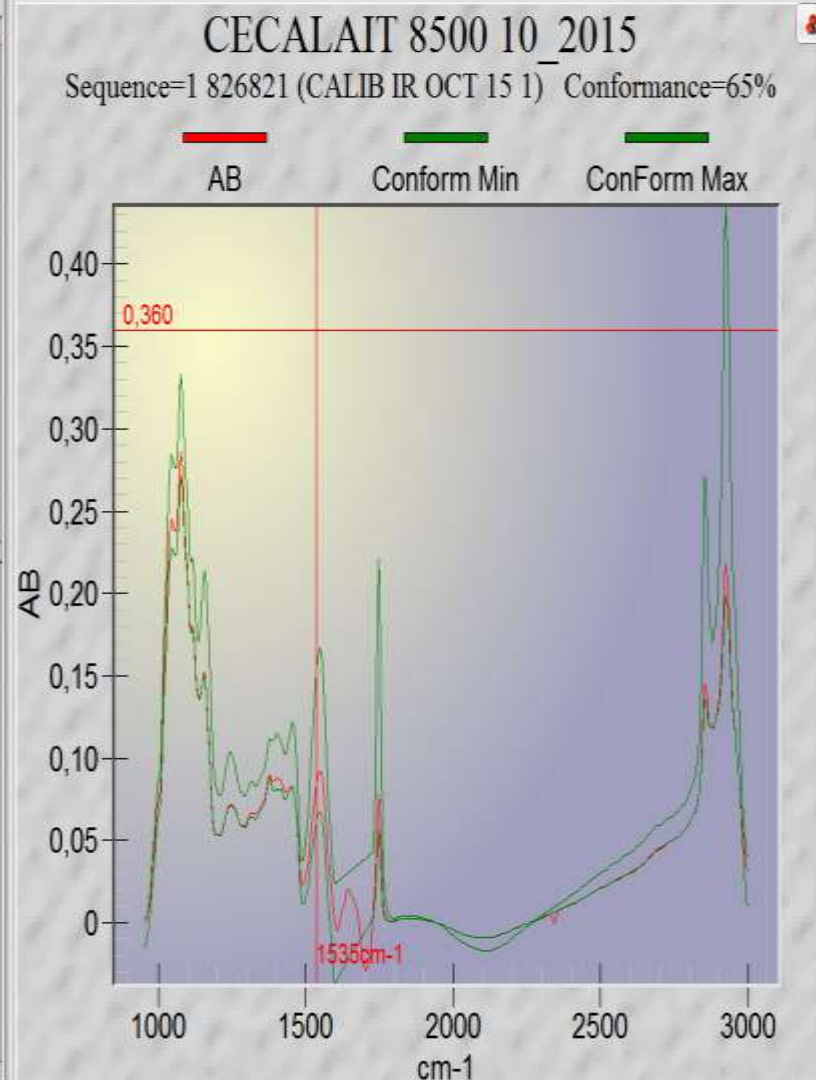


CECALAIT Milk BHB Calibration samples analyzed over 12 months – single calibration, no adjustment required





927960	- R: S: 9 MG 51,38 MP 23,53 Lact 46,11 Urée 10,9 Red	0
927961	- R: S: 9 MG 51,49 MP 23,53 Lact 46,20 Urée 10,9 Red	0
927962	- R: S: 10 MG 36,73 MP 23,56 Lact 47,14 Urée 8,9 Red	0
927963	- R: S: 10 MG 36,79 MP 23,62 Lact 47,21 Urée 8,6 Red	0
927964	- R: S: 11 MG 21,46 MP 31,13 Lact 49,01 Urée 7,3 Red	0
927965	- R: S: 11 MG 21,49 MP 31,23 Lact 49,10 Urée 7,2 Red	0
927966	- R: S: 12 MG 21,58 MP 38,64 Lact 49,00 Urée 7,8 Red	0
927967	- R: S: 12 MG 21,68 MP 38,84 Lact 49,11 Urée 7,4 Red	0



Bentley IR Cell and Spectra standardization
A new highly effective and simple approach (patented)

- Standardization of spectrum x axis with polystyrene NIST international standard
- Standardization of spectrum y axis (absorbance) - patented
- Standardization of all operating conditions and sample preparation
- Removal of any moisture in optical deck that could affect the spectra

Our unique approach leads to real time, optimum and cost effective:

- **Spectra standardization**
- **Calibrations transfer, accuracy and stability**





Thank you for your attention!

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www.bentleyinstruments.com

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