New Technology in NIR Spectroscopy

Rachael Glenister and Bethany Steevens
IAOM, 2017

- *"Unity Scientific was founded to focus on customer satisfaction and technical expertise. We knew that if we took care of the customer and treated them with respect, our technology would find a home, and our value would keep us there." – Doug Evans*

Doug Evans
President and Founder

After completing his marketing degree at the Virginia Polytechnic Institute, Doug started his career in 1979 at Neotec, the original scanning NIR company. For the next 23 years, he held various executive sales and marketing positions with Technicon, Perstorp Analytical, FOSS NIRSystems, and Bran + Luebbe before starting Unity Scientific in 2002.
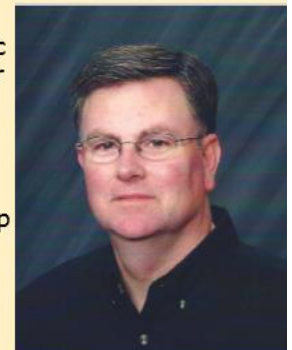
- Completely new and updated system
  - TAS Calibrated
  - Re-designed hardware
 - New UScan software

TAS™

- Total Alignment Spectrometer
- TAS is a patented method for calibrating and maintaining instruments using primary, NIST traceable standards
- A set of 3 TAS standards is measured on your instrument in the factory and at install
- TAS can be run at any time to recalibrate and align your instrument back to "factory specification"

POWERED BY **TAS**

TRUEAlignment™
SPECTROSCOPY

Patents Pending
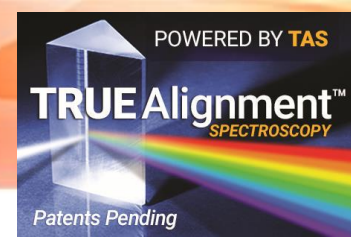
- Guarantees the instrument is always in factory spec!
  - Eliminates possible instrument drift→ Eliminates bias adjustments

- Automatically diagnoses and fixes any instrument alignment issue

- Returns instrument to factory spec after a lamp change or service
  - **No samples needed for bias adjustments**

- Seamless calibration transfer between instruments

- As all Unity instruments will be TAS calibrated, your data is Future Proof
  - Can be easily transferred across systems and models

Customer Samples on XT Flour Model

#	Ref Moisture	NIR Moisture	Diff	Ref Prot14	NIR Prot14	Diff	Ref Ash14	NIR Ash14	Diff
1	13.10	12.86	0.24	11.49	11.56	-0.07	0.627	0.625	0.002
2	13.00	12.75	0.25	10.99	10.89	0.10	0.620	0.598	0.022
3	12.50	12.80	-0.30	10.87	10.82	0.05	0.616	0.604	0.012
4	12.80	12.83	-0.03	10.61	10.71	-0.10	0.614	0.609	0.005
5	13.20	12.90	0.30	10.97	10.81	0.16	0.569	0.577	-0.008
6	12.90	12.57	0.33	11.27	11.17	0.10	0.543	0.569	-0.026
7	12.90	12.82	0.08	11.23	11.10	0.14	0.537	0.574	-0.037
8	13.10	13.29	-0.19	10.26	10.17	0.09	0.510	0.517	-0.007
9	12.60	12.97	-0.37	10.54	10.61	-0.07	0.623	0.615	0.008
10	13.50	13.25	0.25	10.60	10.68	-0.08	0.553	0.564	-0.011
11	13.00	13.09	-0.09	10.47	10.29	0.18	0.510	0.518	-0.008
12	13.55	13.48	0.07	11.12	11.11	0.01	0.541	0.523	0.018
13	13.48	13.51	-0.03	11.38	11.36	0.02	0.535	0.534	0.001
14	13.51	13.42	0.09	11.42	11.41	0.01	0.531	0.534	-0.003
15	13.17	13.36	-0.19	13.62	13.72	-0.10	0.554	0.581	-0.027
16	13.57	13.63	-0.06	11.29	11.31	-0.02	0.520	0.501	0.019
17	13.20	13.39	-0.19	12.64	12.64	0.00	0.542	0.54	0.002
18	13.37	13.34	0.03	10.99	11.14	-0.15	0.523	0.515	0.008
19	13.25	13.15	0.10	10.51	10.60	-0.09	0.543	0.535	0.008
	StdDev		0.20	StdDev		0.10	StdDev		0.016

SpectraStar XT Hardware

- **Built-in PC**
  - Modern, Fast Intel PC Board
    - 8 GB RAM
  - Windows 7 Embedded Operating System
    - 64 bit OS
  - Solid State Hard Drive (no moving parts)
    - 220 GB Storage
  - 17 inch high resolution monitor
  - 4 USB ports

- **Benefits**
  - Fast operation and prediction times
  - Analysis time still under 30 seconds
 - Faster boot-up time
  - Current operating system

- **Made in the USA with highest quality components**

- New high performance detector electronics
    - Ultra Cooled, dual stage InGaAs
    - Very low noise
    - Automatic gain adjustment
- New main controller (mother) board
    - Modern design, powerful
    - Self diagnosing
- New high resolution encoder for extremely accurate and precise wavelength registration
    - Self aligning using TAS first principles
- Highest quality optics for **100% transmission of light through the system**

New
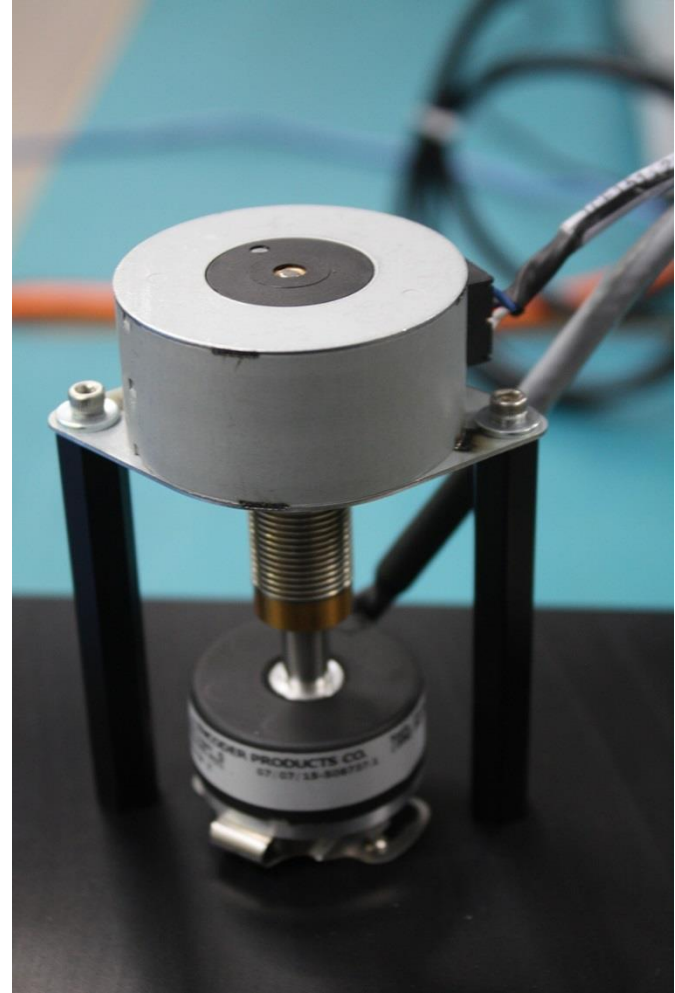
Old

Hardware Features

- **Scans to 2600nm- Higher than any other NIR system!**
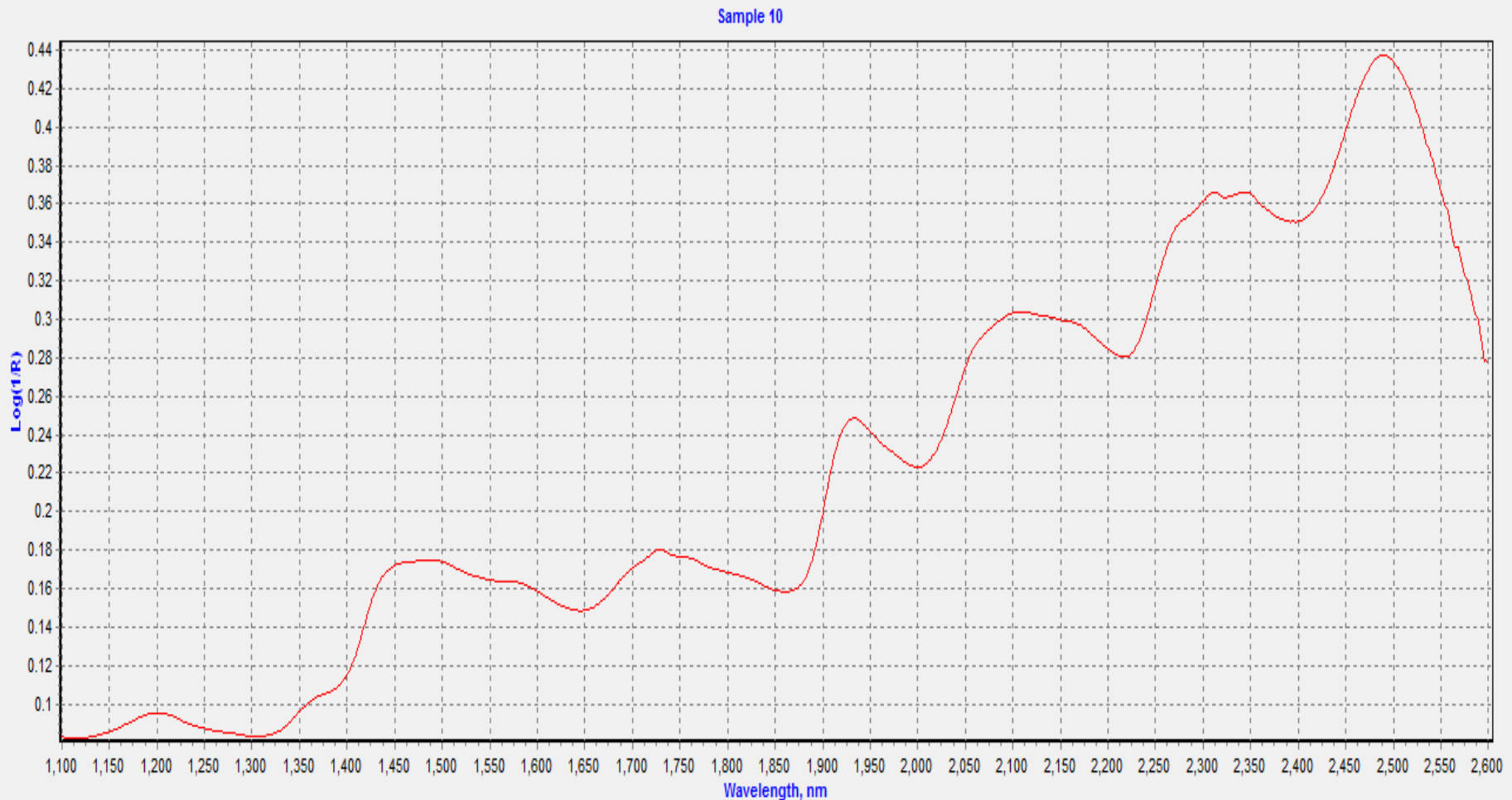
2600 nm Potential Benefits

- Only monochromator to scan to 2600 nm
- This additional information can deliver increased accuracy for constituents containing C-H aromatic and C-N-C amide bonds including
  - Lignin
  - Amino acids
  - Protein
  - Fibers
  - Rheology parameters
- **More information – better results**

- **Best performing system on the market!**
  - ✓ Lowest Noise, RMS < 20 µAU across the entire range

  - ✓ RMS < 15 µAU from 1100-2500 nm

  - ✓ Absolute wavelength accuracy that is best in market

  - ✓ Wavelength precision now similar to FT instruments

- **Best hardware specs lead to most accurate results**

- **Quality = Reliable Performance**

Performance Comparison to NIST

Performance specifications based on the same standards measured at sample plane

Parameter	NEW! Unity SpectraStar XT	Old Unity XL	FOSS DS2500	Bruker Tango
Average Wavelength Difference	0.0151	0.23 nm	0.24 nm	-0.79
Average Absolute Wavelength Difference	0.1877	1.09 nm	0.46 nm	0.95
Wavelength Precision	0.0041	0.23 nm	0.023 nm	0.0004
Average Photometric Difference	0.0010	0.03 Au	0.005 A	-0.220
Average Absolute photometric Difference	0.0011	0.05 Au	0.005 A	0.250
Photometric precision (full scan range)	10.6 µRMS	45 µRMS	42 µRMS	125 µRMS

Unity XL in 2014

Table 2. Performance comparison of multiple commercial instruments

(identical tests and samples)

Parameter	SpectraStar 2500XL-R	Foss NIRS™ DS2500	Bruker Tango	Büchi NIRFlex N-500
λ_{nm} Accuracy [1a]	-0.40	-1.43	-0.31	-1.23
λ_{nm} Accuracy [1b]	-0.79	-5.14	-3.38	-2.25
λ_{nm} Accuracy [2]	-0.23	0.36	-0.79	-0.71
λ_{nm} Precision [1c]	0.014	0.023	0.000	0.048
Photo Accuracy [3]	0.04	-0.005	-0.220	-0.126
Photo Precision [3]	35e-5	13.7e-5	125e-5	75.7e-5
Linearity (R^2) [1d]	0.993	0.976	0.991	0.966
Ave. Stray Light [1d]	1.3%	1.0%	0.20%	4.5%
Noise 680-2500 [3]	66e-6	61e-6	NA	NA
Noise 1100-2500 [3]	19e-6	42e-6	518e-6	168e-6
Noise 1500-2500 [3]	13e-6	45e-6	583e-6	135e-6
Noise 2350-2500 [3]	24e-6	57e-6	816e-6	79e-6
S/N 680-2500 [3]	15133	15933	NA	NA
S/N 1100-2500 [3]	52925	22689	1446	5952
S/N 1500-2500 [3]	74254	21618	1285	7407
S/N 2350-2500 [3]	41286	16937	918	12658

[1a] (3 Wavelength Standard - R99Polystyrene, 10 nm bandwidth), [1b] (8 Wavelength Standard - R99Polystyrene, 10 nm bandwidth), [1c] (2 Wavelength Standard - R99Polystyrene, 10 nm bandwidth), [2] (11 Wavelength Standard - SRM 1920a, 10 nm bandwidth), [1d] (Effective stray light for 5 peak heights using Standard - R99Polystyrene),

[3] (Reflectance/photometric standard - R99, RMS and S/N are for 3 static replicates),

New Unity SpectraStar XT in 2017

Table 2. Performance comparison of multiple commercial instruments

(identical tests and samples)

Parameter	SpectraStar 2500XT-R	SpectraStar 2500XL-R	Foss NIRS™ DS2500	Bruker Tango	Büchi NIRFlex N-500
λ_{nm} Accuracy [1]	0.015	-0.23	0.36	-0.79	-0.71
λ_{nm} Precision [2]	0.005[1]	0.014	0.023[2a]	0.000[2a]	0.048[2a]
Photo Accuracy [3]	0.001	0.04	-0.005	-0.220	-0.126
Photo Precision [3]	10.6e-6[4]	35e-5	13.7e-6	125e-6	75.7e-6
Linearity ($R^{\wedge}2$) [2b]	0.980	0.993	0.976	0.991	0.966
Ave. Stray Light [2b]	0.5%	1.3%	1.0%	0.20%	4.5%
Noise 680-2600 [3]	10e-6[4]	NA	NA	NA	NA
Noise 680-2500 [3]	10e-6[4]	66e-6	61e-6	NA	NA
Noise 1100-2500 [3]	8e-6[4]	19e-6	42e-6	518e-6	168e-6
Noise 1500-2500 [3]	8e-6[4]	13e-6	45e-6	583e-6	135e-6
Noise 2350-2500 [3]	10e-6[4]	24e-6	57e-6	816e-6	79e-6
S/N 680-2500 [3]	100000	16133	15933	NA	NA
S/N 1100-2500 [3]	125000	52925	22689	1446	5952
S/N 1500-2500 [3]	125000	74254	21618	1285	7407
S/N 2350-2500 [3]	100000	41286	16937	918	12658

[1] (11 Wavelength Standard - SRM 1920a, 10 nm bandwidth),

[2a] (2 Wavelength Standard - R99Polystyrene, 10 nm bandwidth),

[2b] (Effective stray light for 5 peak heights using Standard - R99Polystyrene),

[3] (Reflectance/photometric standard - R99, RMS and S/N are for 3 static replicates),

[4] With wavelength range to 2600 nm, static sample.
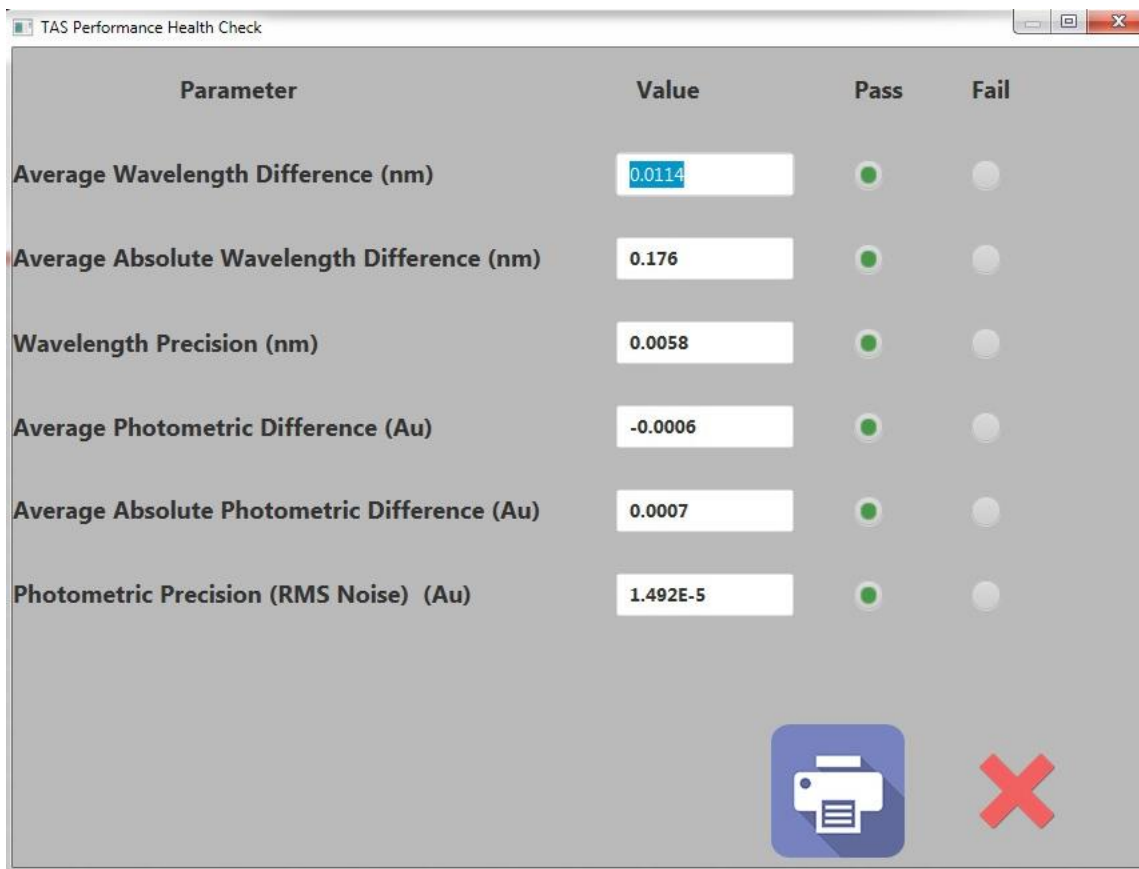
UScan Software

- Completely re-designed software
- Operator-friendly
- Database driven
- New data reporting features
  - ✓ SPC charting
  - ✓ Customers can create customized reports for C of A
- Full, continuous instrument health diagnostics
- Audit friendly
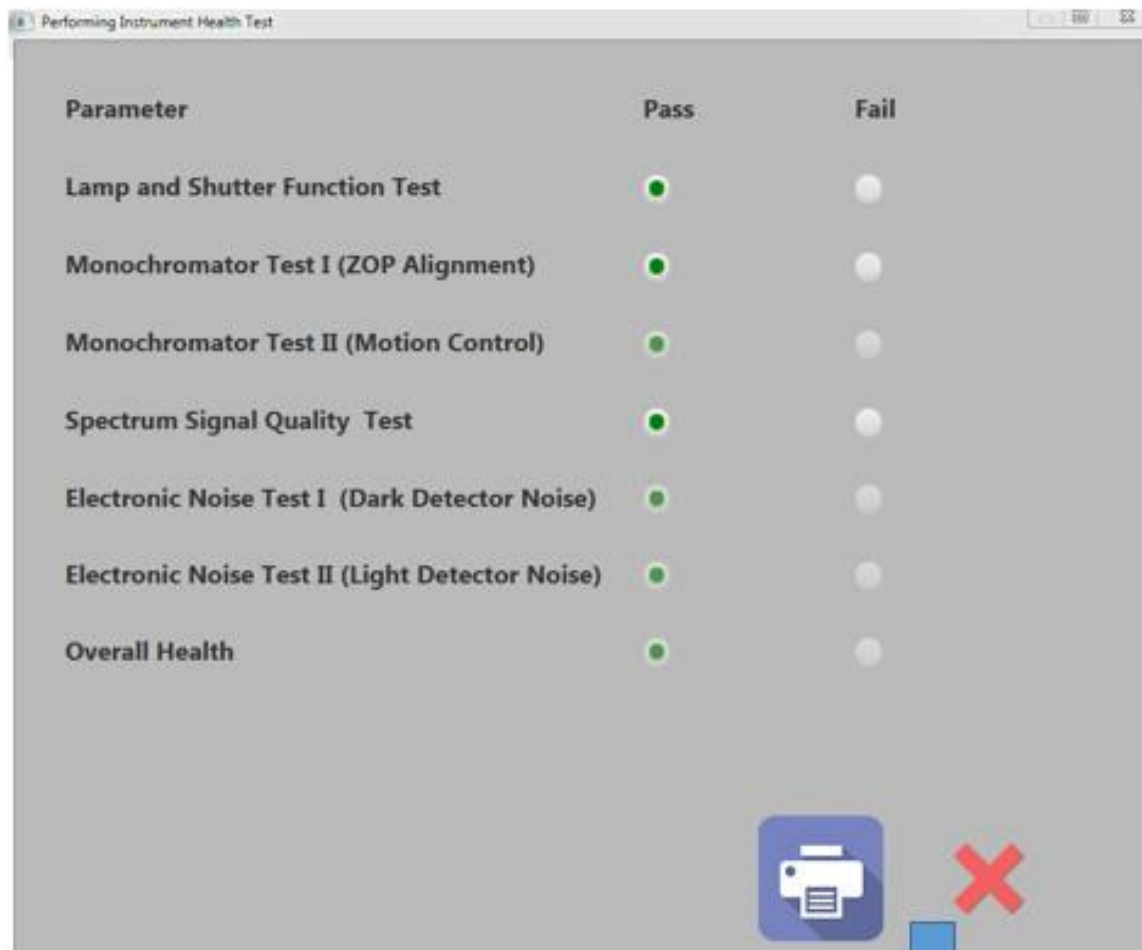
- Built in diagnostics
  - TAS diagnostics to show and verify performance

TAS Performance Health Check

Parameter	Value	Pass	Fail
Average Wavelength Difference (nm)	0.0114	●	○
Average Absolute Wavelength Difference (nm)	0.176	●	○
Wavelength Precision (nm)	0.0058	●	○
Average Photometric Difference (Au)	-0.0006	●	○
Average Absolute Photometric Difference (Au)	0.0007	●	○
Photometric Precision (RMS Noise) (Au)	1.492E-5	●	○

- Built in diagnostics
  - Instrument health to test hardware function and electronics

- Built in diagnostics
  - Lamp health to show lamp quality and predict when change is needed

- When a performance test fails, simply run the TAS procedure and the instrument will **correct, align, and test itself automatically!**

- With the lamp health monitoring, the instrument will **recommend when the lamp needs to be changed**

Instrument Maintenance

- Very easy
- To run diagnostics, just press the button and follow the instructions
- Use TAS to keep the instrument continuously calibrated to factory spec
- 3 new certified standards

Part Number	Description
US-STDS-0004	TAS Photometric Certified Standard
US-STDS-0005	TAS Wavelength Certified Standard
US-STDS-0006	TAS Dark Certified Standard

- The lamp is the same as all other SpectraStars
  - Efficient 5W design
  - Use Lamp Health to monitor the lamp performance

- **No air filter or fan- completely sealed design!**
  - Product of efficient lamp design
  - **We are the ONLY instrument with this feature!**

- New outer case
  - Bright white paint with smooth finish
  - Easy to clean (dry cloth or water/alcohol mix)

- The SpectraStar XT series is rated as IP-52
  - Dust and Moisture protection

- As an upgrade, we can make the system IP-65
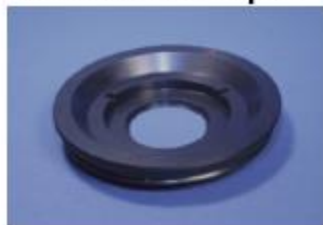 - Ingress protection against all dust and high pressure jets of water

- Flexible Sample Handling
  - Sample Cups – A wide range including FOSS ring cups
  - Petri Dishes
  - Bags
  - Beakers/Vials
  - Heated Flow Cell

- Rotating sample cup for Unground, Partially Ground Samples, or Powders
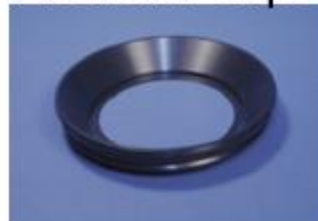 - Most commonly used

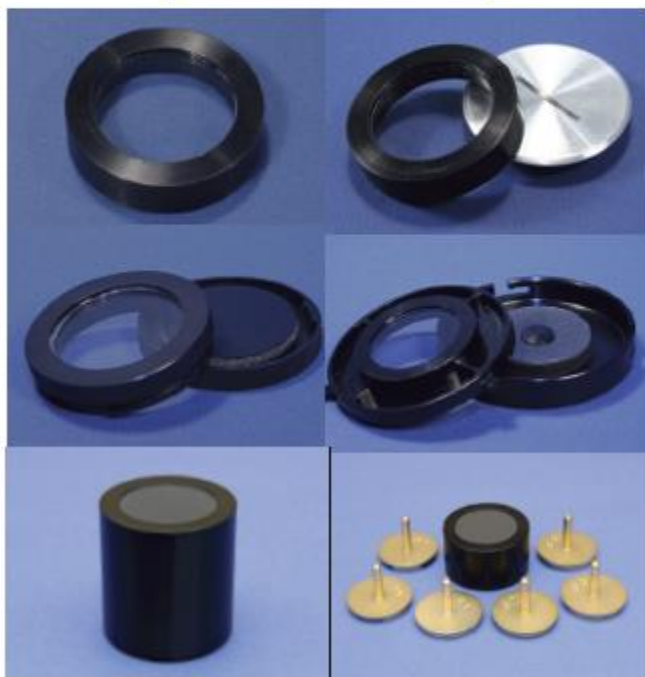- Static for Ground Homogenous Samples

Flexible Sample Handling

- We can transfer database from your previous NIR platform
    - ✓ FOSS
    - ✓ Perten
    - ✓ Bruker
    - ✓ Buchi

Seeking New Applications?

Wheat Flour					
Parameter	N	RSQ	MIN	MAX	SECV
Moisture	1469	0.895	11.9	15.1	0.10
Protein	1588	0.993	5.3	15.74	0.17
Ash	1521	0.853	0.27	0.68	0.017
Alveograph - P	514	0.808	17	41.5	2.28
Alveograph - W	531	0.815	30	120	8.23
Color - B	1088	0.937	78.26	88.19	0.436
Water Absorption	1194	0.937	46.9	75.2	1.04
Farinograph - Development Time	1123	0.901	0.7	8	0.63

- Starch damage
- Gluten

- TAS calibrated for stability and future proof data
- Easy, robust, and low maintenance
- Completely re-designed hardware
- New UScan software
- Best performance on the market!

Alveolab

Amylab FN

Labmill

SRC

Mixolab