Applied NIR Spectroscopy Workshop: From Theory to Calibration and Instrumentation

Seminar Room, Plant Science Building, NC State University, Raleigh, North Carolina, USA

November 9 to 11, 2026

Workshop Modules

1. The Basics of NIR and Trends
2. Open-source Chemometrics for NIR Spectroscopy
3. Applications, Model Life-cycle Assessment, Transferability

Workshop Facilitators

Miguel S. Castillo, NC State University
Juan J. Acosta, NC State University
Marçal Plans, Buchi
Leonardo Ramirez-Lopez, Buchi
Matthew Eady, Orion RTP

Logistics (contact info)

Bessy Santos Velasquez (braudal@ncsu.edu ; 919-444-5189)
Amber Polk
Lauren Rouse

The schedule is set up with four training sessions each day, two sessions in the morning and two in the afternoon.

Day 1, November 9
The Basics of NIR and Trends

Time	Activity/Topic
08:30 – 09:00	Breakfast, registration, and welcoming remarks
09:00 – 10:40	Session 1: NIR Theory • Electromagnetic spectrum and molecular vibrations • Functional groups and light scattering
10:40 – 10:50	Coffee break
10:50 – 12:30	Session 2: Parts of the NIR instrumentation and types of spectrometers • Light-matter interactions • Instrumentation and components • Resolution and signal-to-noise • Sampling considerations
12:30 – 13:30	Lunch break
13:30 – 15:10	Session 3: New trends in NIR technology • Components, miniaturization • Benchtop versus portable spectrometers • Software and data, business models
15:10 – 15:20	Coffee break
15:20 – 17:00	Session 4: Where we can find NIR • Classical NIR applications • New application fields for NIR • Next generation (data fusion, self-maintaining models, remaining challenges)

Day 2, November 10
Open-source Chemometrics for NIR Spectroscopy

Time	Activity/Topic
08:30 – 09:00	Breakfast
09:00 – 10:40	Session 1: Introduction to Chemometrics and R Programming. • Basics of Chemometrics Modeling • R programing
10:40 – 10:50	Coffee break
10:50 – 12:45	Session 2: NIR Modeling Using R. • Transformations and outliers • Model Selection • Prediction
12:45 – 13:30	Lunch break
13:30 – 15:10	Session 3: Chemometrics Pipeline • Chemometrics pipeline overview: from spectral data to a deployable model • Import and Inspect: load spectra and reference values; explore calibration and validation datasets • Preprocess: combine spectral treatments into reusable recipes
15:10 – 15:20	Coffee break
15:20 – 17:30	Session 4: Chemometrics Pipeline – cont. • Calibrate: build PLS models and select settings through cross-validation • Validate: predict independent samples and interpret performance • Deploy: export the model for an instrument and use it • Review and questions
18:30 – 20:30	Social activity

Day 3, November 11
Applications, Model Life-cycle Assessment, Transferability

Time	Activity/Topic
08:30 – 09:00	Breakfast
09:00 – 10:40	Session 1: Pharmaceutical Applications • Qualitative analysis in finished pharmaceutical product supply chains • Quantitative applications in pharmaceutical quality control
10:40 – 10:50	Coffee break
10:50 – 12:30	Session 2: Model life-cycle assessment and transferability • Practical guidelines for maintaining and updating models • Exporting and deploying NIR models • Calibration transfer strategies
12:30 – 13:30	Lunch break
13:30 – 15:00	Session 3: Target-domain sample selection • Identifying the most relevant samples within large datasets • Building robust calibration models using selected subsets
15:00 – 16:00	Session 4: Closing thoughts • Experiment-Specific NIR models • Validation
16:00 – 17:00	Coffee break, END

ADDITIONAL NOTES

Name badges can be pick up at registration. Please wear your badges every day.

Breakfast, lunch, and two coffee breaks are included each day.

A social event is scheduled on Tuesday (November 10), after the workshop, and we cordially invite you attend. Hors d'oeuvres will be provided at a reserved location.