

NIR Spectroscopy Quick Reference Guide

NIR Fundamentals Course | Instructor: Vitaly Kirkpatrick

A concise reference for essential NIR spectroscopy concepts, formulas, and specifications.

Wavelength Ranges

Region	Range (nm)	Description
Visible	400-780	Human eye sensitivity
NIR (Near-Infrared)	780-2500	Standard NIR definition
Extended NIR	400-2500	Modern dual/triple detector systems
SWIR (Short-Wave IR)	780-1100	Silicon detector range
Mid-IR	2500-25000	Fundamental vibrations

Detector Specifications

Single-Detector Systems

- **Silicon (Si):** 400-1100 nm (visible + SWIR)
- **InGaAs:** 900-1700 nm (most common NIR)
- **PbS:** 1000-2500 nm (extended NIR, cooled)

Dual-Detector Systems

- **Si + InGaAs:** 400-1700 nm

- Overlap region: 900-1100 nm
- Most common for extended-range instruments

Triple-Detector Systems

- **Si + InGaAs + PbS:** 400-2500 nm
- Full visible-NIR coverage
- High-end laboratory instruments

Key Formulas

Beer-Lambert Law

$$A = \epsilon \times b \times c$$

Where:

A = Absorbance (no units)

ϵ = Molar absorptivity ($\text{L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$)

b = Path length (cm)

c = Concentration ($\text{mol} \cdot \text{L}^{-1}$)

Transmittance to Absorbance

$$A = -\log_{10}(T)$$

$$T = 10^{-A}$$

Where:

T = Transmittance (fraction, 0-1)

A = Absorbance

Wavelength-Wavenumber Conversion

$$\tilde{\nu} (\text{cm}^{-1}) = 10,000,000 / \lambda (\text{nm})$$

$$\lambda (\text{nm}) = 10,000,000 / \tilde{\nu} (\text{cm}^{-1})$$

Calibration Statistics

R² (Coefficient of Determination)

$$R^2 = 1 - (SS_{\text{res}} / SS_{\text{tot}})$$

Interpretation:

> 0.95 = Excellent

0.90-0.95 = Very good

0.80-0.90 = Good

< 0.80 = Poor

RMSE (Root Mean Square Error)

$$RMSE = \sqrt{(\sum (y_{\text{pred}} - y_{\text{true}})^2 / n)}$$

Lower is better

Should be small relative to measurement range

RPD (Ratio of Performance to Deviation)

$$RPD = SD_{\text{ref}} / RMSEP$$

Interpretation:

> 4.0 = Very good (reliable quantitative QC)

3.0-4.0 = Good (quality control)

2.0-3.0 = Poor to approximate (screening only)

< 2.0 = Not suitable

Bias

$$\text{Bias} = \sum (y_{\text{pred}} - y_{\text{true}}) / n$$

Should be close to zero

Positive = overestimation

Negative = underestimation

Functional Groups & NIR Absorption

Functional Group	Wavelength (nm)	Type	Common Applications
O-H (water)	1450, 1940	1st & 2nd overtone	Moisture analysis
O-H (alcohol)	1400-1500	1st overtone	Alcohol content
N-H (protein)	1500, 2050	1st & 2nd overtone	Protein analysis
C-H (fat)	1200, 1730	2nd & 3rd overtone	Fat/oil content
C-H (aromatic)	1680-1780	Combination	Aromatic compounds
C=O	2100-2200	Combination	Carbonyl groups

Preprocessing Methods

Derivative Spectroscopy

- **1st Derivative:** Removes baseline offset, enhances peaks
- **2nd Derivative:** Removes linear baseline, enhances fine structure
- **Savitzky-Golay:** Smoothing + derivative calculation

Scatter Correction

- **MSC (Multiplicative Scatter Correction):** Corrects for light scattering
- **SNV (Standard Normal Variate):** Centers and scales each spectrum

Other Methods

- **Baseline Correction:** Removes systematic baseline drift
- **Normalization:** Scales spectra to common reference
- **Smoothing:** Reduces high-frequency noise

Instrument Types

Dispersive Instruments

- Use diffraction grating to separate wavelengths
- Sequential wavelength scanning
- Typical range: 400-2500 nm
- Advantages: Simple, robust, cost-effective
- Disadvantages: Slower than FT-NIR

FT-NIR (Fourier Transform)

- Use interferometer (Michelson)
 - Simultaneous measurement of all wavelengths
 - Typical range: 800-2500 nm
 - Advantages: High speed, high SNR, wavelength accuracy
 - Disadvantages: More complex, higher cost
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Sampling Modes

Mode	Description	Applications
Diffuse Reflectance	Light scattered from sample surface	Powders, solids, slurries
Transmittance	Light passes through sample	Liquids, thin films
Transflectance	Transmission + reflection	Liquids in vials, tablets
Interactance	Short path diffuse transmission	Thick samples, fruits

Model Validation Guidelines

Calibration Set

- Minimum 50-100 samples (more is better)
- Cover full range of variation
- Representative of population
- Accurate reference values

Validation Set

- Independent from calibration
- 20-30% of total samples
- Cover full range
- Test model performance

Cross-Validation

- Leave-one-out (LOO)
- K-fold (typically 5-10 folds)
- Estimates prediction error
- Use when validation set is limited

Troubleshooting Quick Guide

Problem	Possible Causes	Solutions
Poor R ²	Insufficient samples, poor reference data, wrong preprocessing	Add samples, verify reference method, try different preprocessing
High RMSE	Model overfitting, outliers, sample heterogeneity	Reduce model complexity, remove outliers, improve sampling
High Bias	Calibration drift, temperature effects, reference method bias	Recalibrate, control temperature, verify reference method
Low RPD	High noise, insufficient spectral variation	

Problem	Possible Causes	Solutions
		Increase scan averaging, expand calibration range
Outliers	Sample contamination, measurement error, unusual samples	Investigate and remove if justified

Industry Applications

Food & Agriculture

- Moisture, protein, fat, fiber
- Quality grading
- Adulteration detection
- Process monitoring

Pharmaceuticals

- API content
- Blend uniformity
- Tablet coating
- Raw material ID

Process Monitoring

- Real-time quality control
- Batch release testing
- In-line measurements
- Process optimization

Professional Organizations

- **CNIRS:** Council for Near-Infrared Spectroscopy

- **IDRC:** International Diffuse Reflectance Conference
 - **SAS:** Society for Applied Spectroscopy
 - **ACS:** American Chemical Society
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Key Journals

- Journal of Near Infrared Spectroscopy (JNIRS)
 - Applied Spectroscopy
 - Talanta
 - Analytica Chimica Acta
 - Spectroscopy Online (industry news)
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Common Mistakes to Avoid

1. ❌ Using too few calibration samples
 2. ❌ Ignoring outliers without investigation
 3. ❌ Overfitting models (too many latent variables)
 4. ❌ Not validating with independent samples
 5. ❌ Poor sample presentation/preparation
 6. ❌ Ignoring temperature effects
 7. ❌ Not maintaining instrument calibration
 8. ❌ Using inappropriate preprocessing
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Best Practices

1. ✅ Collect representative calibration samples
2. ✅ Use accurate reference methods
3. ✅ Control sample temperature
4. ✅ Standardize sample presentation

5.  Validate models regularly
 6.  Monitor model performance over time
 7.  Document all procedures
 8.  Train operators properly
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For detailed explanations, see course lessons and glossary.