METASPEQ

Near-Infrared Spectroscopy

APPLICATION NOTE

Uniformity of content testing of Paracetamol Tablets Using NIR Spectroscopy and chemometric analysis

MetaspeQ™ near-infrared spectrometers, use proprietary AI/ML technology, **SpectraFind™**, as a cost-effective, rapid, and reliable alternative to HPLC for accurate paracetamol content testing, ensuring efficient quality control in tablet production.



AT A GLANCE

Challenges

- Time-consuming sample preparation process.
- Requires expensive solvents and reagents.
- Complex and labor-intensive procedures.

Benefits

- Significant cost savings.
- Drastically reduces analysis time.
- Eliminates need for sample preparation.
- Accurate content quantification achieved.



OBJECTIVES

Assess Paracetamol Content Accuracy- Evaluate the accuracy of paracetamol content in tablets using NIR spectroscopy combined with advanced preprocessing techniques.
Compare accuracy and efficiency to benchmark- Compare the effectiveness, cost, and time efficiency of NIR spectroscopy versus traditional HPLC methods.
Validate Robustness of Chemometrics model- Validate the effectiveness of SpectraMax™ preprocessing techniques in enhancing NIR spectral analysis for reliable quantification.

SOLUTIONS

Advanced AI/ML significantly enhanced the performance of PLSR in analyzing paracetamol samples indicated a strong correlation between predicted and actual values (HPLC results). The model also achieved low Root Mean Square Error (RMSE) values (0.39 for calibration and 0.41 for prediction), reflecting minimal prediction errors. Additionally, high Residual Predictive Deviation (RPD) values confirm the robustness of this approach, making it highly effective for accurate and reliable quantification of paracetamol.

BENEFITS

Enhanced Analysis Speed and Efficiency: Achieve up to 90% reduction in analysis time and costs while maintaining high accuracy and reliability.
Non-Destructive Testing Method : Conduct analysis without destroying samples, allowing for more efficient use of resources and preserving tablet integrity.
Cost-Effective Quality Control- Reduce the need for expensive reagents and solvents, lowering overall operational costs while ensuring robust quality control in tablet production.

NEXT-GENERATION QUALITY ANALYSIS

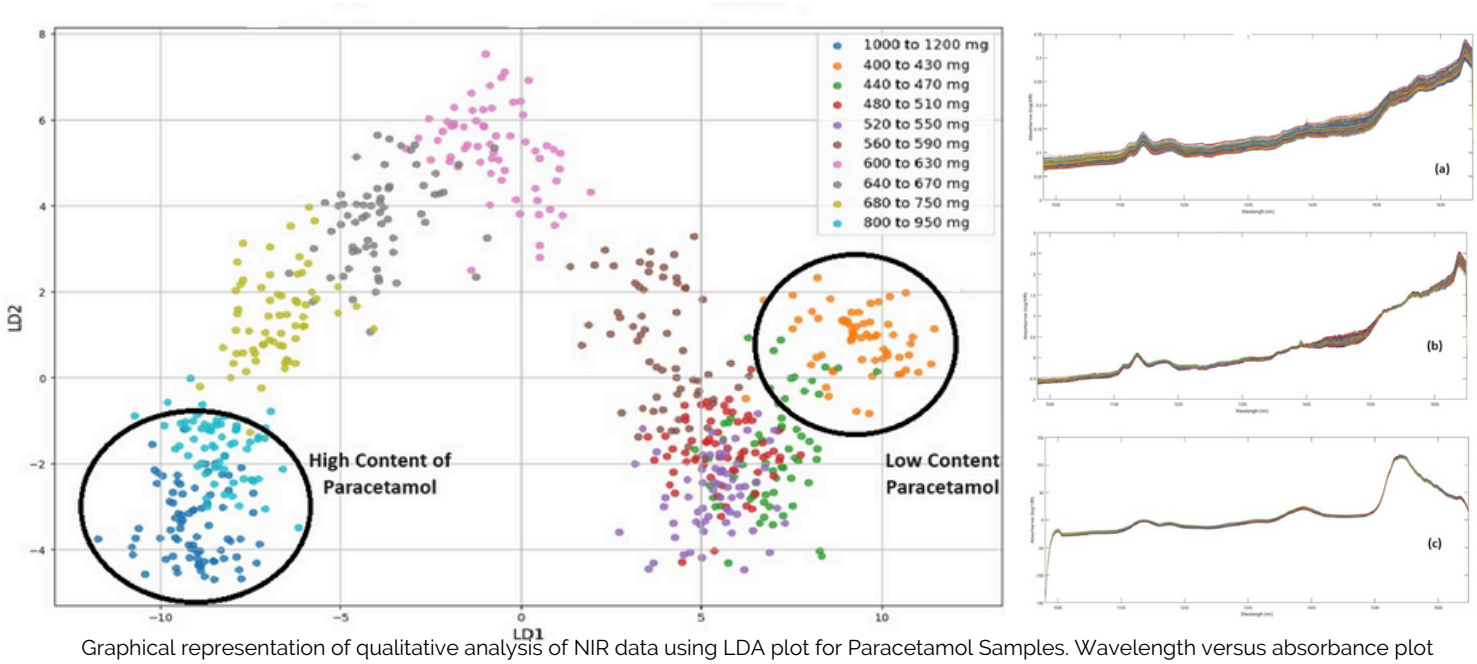
STUDY BRIEF

METHODS

Paracetamol tablets were analysed using Metaspeq™ NIR spectroscopy, with samples prepared by mixing paracetamol IP powder (400-1200 mg) and excipients with a constant amount of excipients to prepare the representative tablet samples for NIR analysis. HPLC analysis of the paracetamol powder to check the purity based on the IP-based method (methanol/water/O-phosphoric acid (40 + 60 +0.05 v/v)). Spectral data were acquired using a Metaspeq™ NIR spectrometer and analyzed with SpectraFInd software. Preprocessing techniques like SNV and Savitzky-Golay filtering were applied to ensure accurate, non-destructive content analysis.

RESULTS AND DISCUSSION

Linear Discriminant Analysis (LDA) -The LDA plot graphically represents the qualitative analysis of NIR data for paracetamol samples with varying mg contents. LD1, which captures 84.31% of the variance, strongly distinguishes between different mg contents, while LD2, accounting for 11.45% of the variance, further separates the groups. This visualization aids in understanding and classifying the data's distribution and relationships.



Graphical representation of qualitative analysis of NIR data using LDA plot for Paracetamol Samples. Wavelength versus absorbance plot (a) Raw data (b) SNV data (c) the SNV+ SG pre-processed spectra of Paracetamol Sample

The application of SpectraFind preprocessing techniques significantly enhanced the performance of PLSR in analyzing paracetamol samples. The PLSR model demonstrated high R^2 values, with 0.913 for calibration and 0.965 for prediction, indicating a strong correlation between predicted and actual values. The model also achieved low Root Mean Square Error (RMSE) values (0.39 for calibration and 0.41 for prediction), reflecting minimal prediction errors. Additionally, high Residual Predictive Deviation (RPD) values confirm the robustness of this approach, making it highly effective for accurate and reliable quantification of paracetamol.

Pre-Processing	Calibration			Prediction		
	R2c	RMSEc	RPDc	R2p	RMSEp	RPDp
None	0.90	0.49	4.45	0.88	0.51	3.01
S.N.V.	0.910	0.42	4.91	0.935	0.45	3.9
SpectraFind	0.913	0.39	5.43	0.965	0.41	3.22

TAKEWAY

MetaspeQ™ NIR with SpectraFind™ offers rapid, cost-effective paracetamol tablet testing, replacing HPLC, reducing costs by 90%, and ensuring precise, non-destructive quality control.