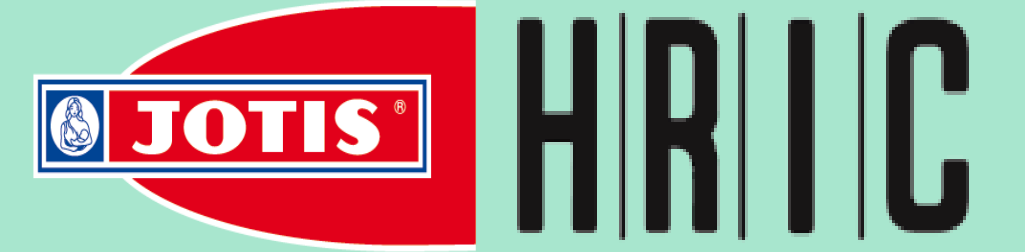


Application of FT-NIR Spectroscopy Coupled with Chemometrics for Rapid Quantification of Macronutrients in Cereal-Based Baby Food

Alexandra Nanou^{1*}, Evangelia Krystalli¹, Sofia Koutroumpi¹

¹Hellenic Research and Innovation Centre, YIOTIS S.A., Athens, Greece

*email: a.nanou@hriclabs.gr, e.krystalli@hriclabs.gr, s.koutroubi@hriclabs.gr



1 INTRODUCTION



The demand for **accurate, efficient, and non-destructive** methods to analyze nutritional components in food products has grown significantly, particularly in the context of **infant nutrition**, where precise nutrient quantification is critical. This study presents the development of a **rapid and cost-effective approach** using **Fourier Transform Near-Infrared (FT-NIR) spectroscopy** combined with **chemometric techniques** to simultaneously quantify key macronutrients in cereal-based baby foods:

- Total sugars (including fructose, glucose, sucrose, maltose, and lactose),
- Protein
- Fat

- This method not only **simplifies the process** of nutrient analysis but also ensures that the **integrity** of the food samples is preserved, addressing industry needs for both **accuracy** and **efficiency** in quality control.
- Most importantly: This study demonstrates a **novel approach** for **simultaneous quantification of critical macronutrients in cereal-based baby foods**, ensuring both safety and nutritional quality for infants

2 SCOPE

This research focuses on establishing an **innovative analytical framework** to quantify **seven primary macronutrients** essential for **infant nutrition**. By employing **FT-NIR spectroscopy**, the study aims to overcome the limitations of traditional chemical analysis methods, which are often time-intensive, destructive to samples, and costly. FT-NIR spectroscopy, in conjunction with chemometric modeling, enables **simultaneous and precise quantification** of target components, making it suitable for high-throughput analysis in food quality control laboratories. This study has the potential to set new standards for **rapid nutrient assessment** in baby food production, ensuring product **consistency and safety**.

3 MATERIALS & METHODS

SAMPLE COLLECTION

158 cereal-based baby food samples



REFERENCE METHODS

Laboratory analyses

HPLC-RID

KJELDAHL

SOXHLET



Total sugars determination

Protein determination

Fat determination

SPECTROSCOPIC ANALYSIS

FT-NIR



Integrating sphere

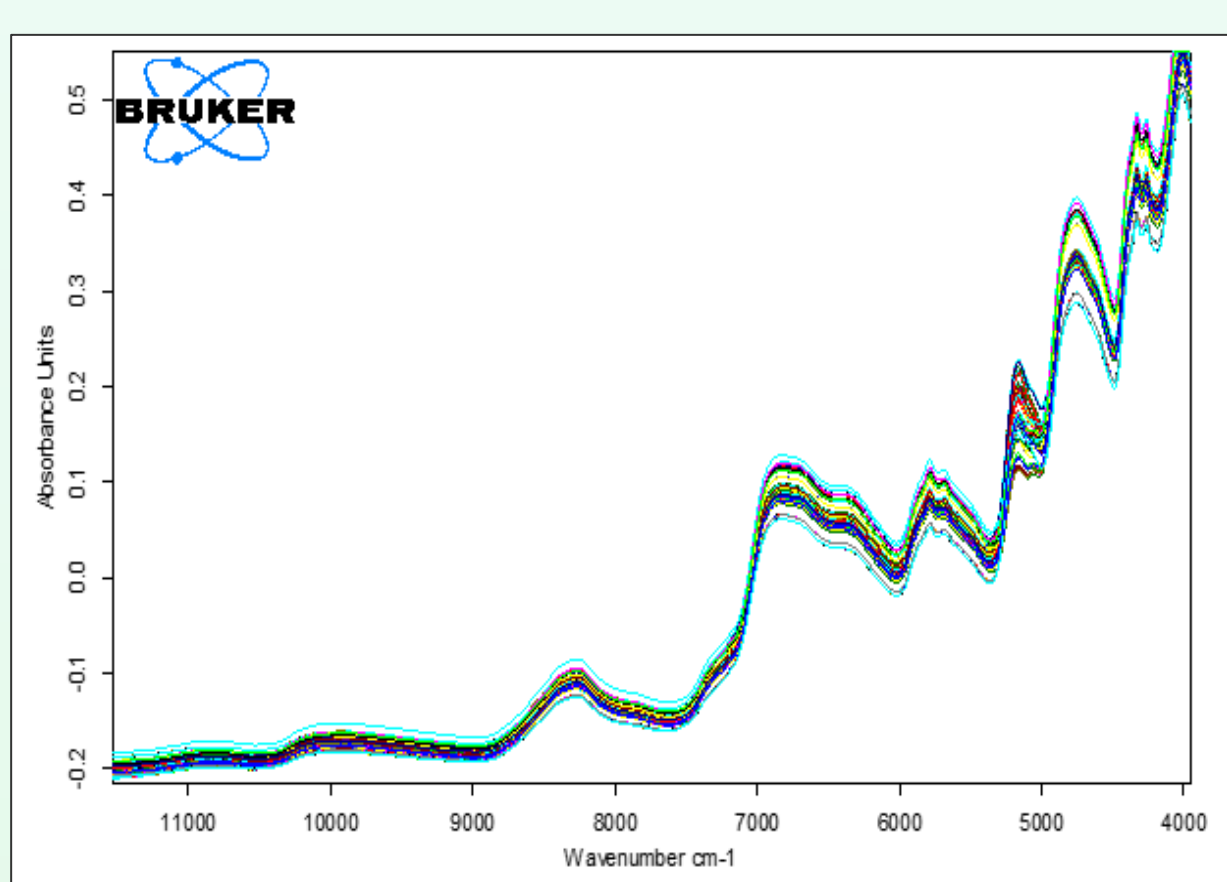


DATA ANALYSIS

- Spectral **pre-processing** → First derivative transformation, Vector normalization, Smoothing
- Combination of spectra with reference values
- Calibration model development:
 - Partial Least Squares Regression (PLSR) used to build robust models for each nutrient (OPUS Spectroscopy Software)
 - **Specific spectral regions** optimized for quantifying individual components
- Model performance assessment evaluated by key metrics:
 - Coefficient of determination (R^2)
 - Root mean square error of calibration (RMSEC)

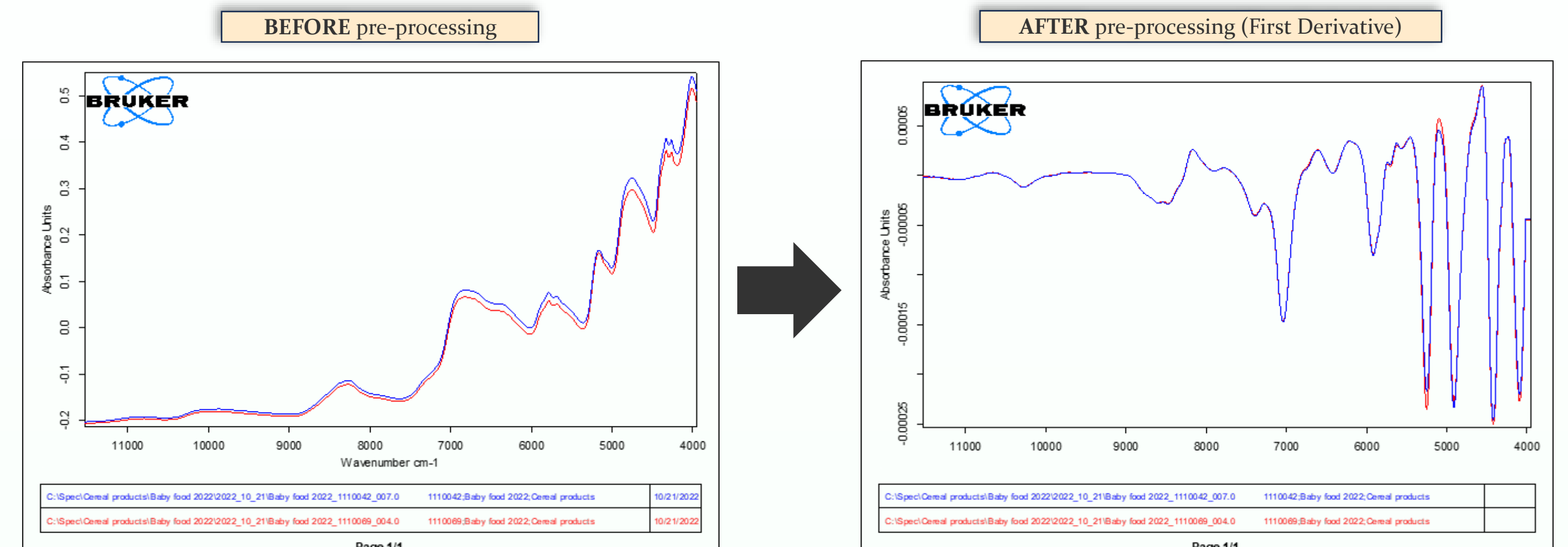
REPRESENTATIVE SPECTRA

Spectral range → 4000 to 12500 cm^{-1}

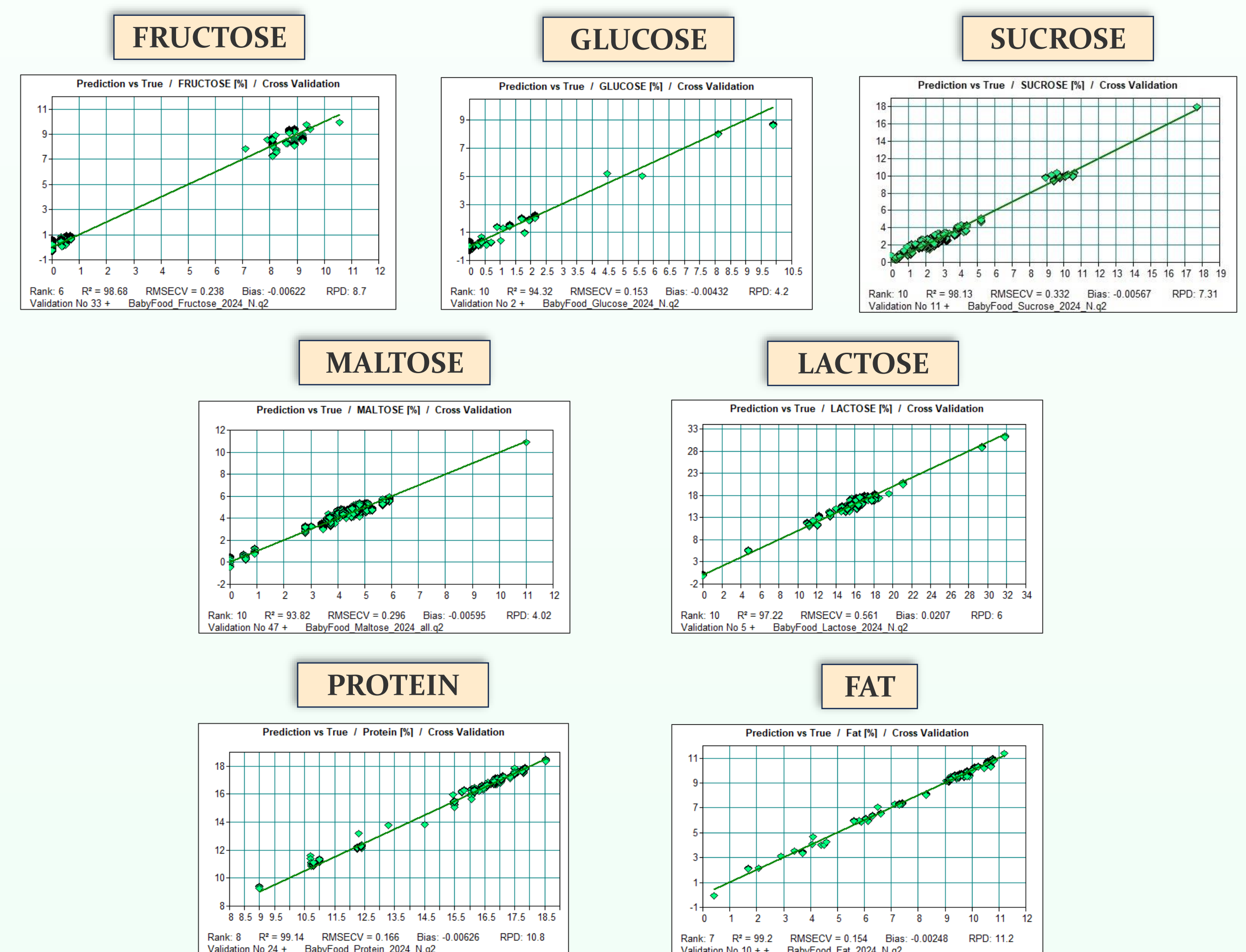


4 RESULTS

Typical IR spectra of baby food



Calibration curves for 7 key macronutrients:



CROSS VALIDATION

	FRUCTOSE	GLUCOSE	SUCROSE	MALTOSE	LACTOSE	PROTEIN	FAT
Spectra	2142	2128	2320	2301	2328	1682	1777
Cal spectra	1200	1660	1115	881	831	635	720
R^2	98,68	94,32	98,13	93,82	97,22	99,14	99,2
RMSECV (Std error)	0,238	0,153	0,332	0,296	0,561	0,166	0,154
Calibration range	0 - 10,57	0 - 9,9	0,0 - 17,7	0 - 11	0,0 - 31,8	9,9 - 18,526	0,41 - 11,2
Rank	6	10	10	10	10	8	7
Spectral Regions	8056-7592 / 6544-6040 / 5024-4496	7608-5328 / 4520-4168	9008-5328 / 5024-4128	8056-5328	5024-4128	8056-7592 / 7144-6040	7144-6536 / 6040-5328 / 5024-4168
Pre-processing	FD	SNV	SNV	FD	FD + SNV	SNV	SNV

**FD: 1st Derivative, SNV: Vector Normalization

EXTERNAL TESTING

10 unknown baby food samples excluded from the calibration data

	TOTAL SUGARS		PROTEIN		FAT	
	AVERAGE	SD	AVERAGE	SD	AVERAGE	SD
HPLC - KJELDAHL - SOXHLET	23,72	1,51	16,97	0,81	9,48	0,15
FT-NIR	23,85	1,44	17,04	0,78	9,49	0,15
DEVIATION	0,5%		0,4%		0,1%	

5 CONCLUSION

- Applicability of **FT-NIR spectroscopy** combined with **chemometric analysis** for reliable **macronutrient quantification** in cereal-based baby foods.
- Validation through **high R^2 values** and **low RMSEC values**, proving the approach to be **accurate and efficient** for determining **protein, fat, and sugar** content.
- **Non-destructive** and **rapid processing** capabilities of FT-NIR make it an effective alternative to traditional chemical methods.
- Ideal for **quality control** in the baby food industry due to its **speed and reliability**.
- FT-NIR spectroscopy is an innovative and practical solution for maintaining high standards of nutritional accuracy in infant food products.