



Data Article

A dataset of visible – Short wave InfraRed reflectance spectra collected on pre-cooked pasta products



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ABSTRACT

Reflectance Visible (Vis) and Short Wave Infrared (SWIR) spectra of pre-cooked pasta products were collected in a non-invasive way by using an ASD FieldSpec® 4 Standard-Res portable spectrophotometer (350–2500 nm). Vis-SWIR data were collected on 6 samples of *Pennette 72* and 6 samples of *Mezze Penne* with different salting levels with the aid of a contact probe in two different physical conditions: i) frozen and ii) thawed. Fifty Vis-SWIR spectra were collected per measurement time from each sample resulting in 1200 raw spectra.

The dataset presented in this descriptor can be used to explore the possibilities to develop automated methods to perform pre-cooked pasta analysis. Vis-SWIR data have potential reuse for follow-up studies finalized to develop pre-cooked

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pasta quality control applications by using similar devices or to test the ability of different chemometric algorithms.

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Specifications Table

Subject	Spectroscopy.
Specific subject area	Biophotonics; food quality control applications.
Type of data	Table (.mat and .csv files).
How data were acquired	Portable Visible (Vis) and Short Wave InfraRed (SWIR) spectroscopy. ASD FieldSpec® 4 Standard-Res field portable spectroradiometer in reflectance mode in the wavelength range of 350–2500 nm with a spectral resolution of 3 nm at 700 nm and 10 nm at 1400/2100 nm, resulting in 2151 variables/measurement.
Data format	Raw data, analysed data.
Parameters for data collection	A Spectralon (reflectance >99%) standard material was used for calibrating the instrument, followed by dark current. Calibration was performed for each cycle of sample acquisition. The analyzed samples consist of two types of pre-cooked pasta, with different degrees of salting - <i>Pennette72</i> and <i>Mezze Penne</i> - in two physical conditions: frozen (just taken out from the dry ice icebox) and thawed (after about two hours left to rest at a temperature of 26 °C).
Description of data collection	Reflectance spectra were acquired with a portable spectroradiometer aided by a contact probe from pre-cooked pasta samples in different physical conditions (being frozen/being thawed). Fifty spectra acquisitions were performed, for each pre-cooked pasta sample, using a portable spectrophotometer, after a specific calibration procedure. The collected data can be imported into MATLAB environment to perform the analysis.
Data source location	Institution: Raw Materials Laboratory, Sapienza University of Rome. City/Town/Region: Latina (LT), Lazio. Country: Italy.
Data accessibility	The datasets described in this paper are hosted in a public repository. Repository name: Bonifazi, Giuseppe; Gasbarrone, Riccardo; Capobianco, Giuseppe; Serranti, Silvia (2021), "A dataset of Visible – Short Wave InfraRed reflectance spectra collected on pre-cooked pasta products", Mendeley Data, V2, doi: 10.17632/yhyzmp8rtb.2 Direct URL to data: http://dx.doi.org/10.17632/yhyzmp8rtb.2

Value of the Data

- The dataset can be used as a reference set of spectral signatures of pre-cooked pasta, and for the development of automated methods of pasta-based products' physical condition evaluation.
- Researchers working with visible and near infrared spectroscopy, especially the reflectance spectroscopy equipment used in combination with food control and pre-cooked pasta products quality inspection will benefit from these data, on a case-by-case basis, and depending on the personal investigation.

Data can be re-used: i) to set up multivariate classification models for discriminating pasta-based products according to their physical condition and ii) to perform multivariate regression for predicting the dry weight content of pre-cooked pasta.

1. Data Description

In recent times, more and more companies working in the pasta sector are starting to use methods based on Near InfraRed (NIR) spectroscopy, combined with chemometrics, allowing quick investigations in order to perform simultaneous determinations of different parameters [1–3].

Visible and NIR spectroscopy techniques are actually utilized to perform both qualitative and quantitative analysis in different fields: i.e. in primary/secondary raw materials sector [4,5], in cultural heritage [6,7], in the agricultural and food industry [8–13], in the pharmaceutical and chemical industry [14,15], in clinical application [16–18] and more generally in analytical science [19] to perform systematic environmental remote and proximal sensing. In this data descriptor, reflectance Visible (Vis) and Short Wave Infrared (SWIR) spectra of pre-cooked pasta products are reported.

Reflectance Vis- SWIR spectra of pre-cooked pasta product were acquired by an ASD FieldSpec® 4 Standard-Res field-portable spectrophotometer (350–2500 nm). Vis-SWIR data were collected on 6 samples of *Pennette 72* and 6 samples of *Mezze Penne* with different salting levels, by the aid of a contact probe, in two different physical conditions: i) frozen and ii) thawed.

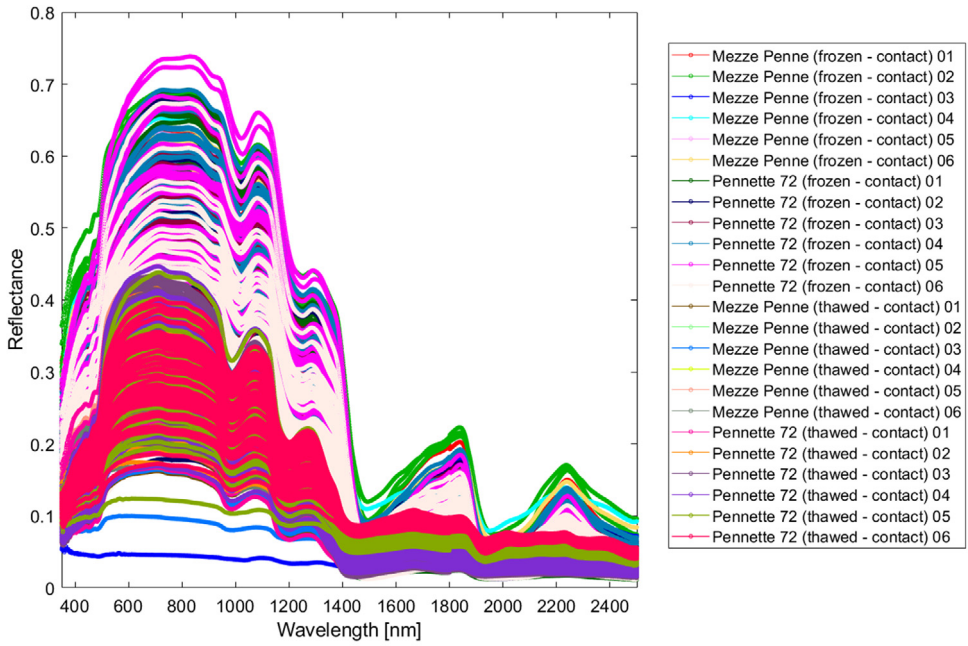
The data records presented in this work are reported in a public repository (i.e. Mendeley Data) and consist of a MATLAB (MathWorks Inc., Natick, MA, USA) “.mat” file. More in detail, the “Pasta_dataset.mat” is a MATLAB data file containing a DataSet Object (DSO), the “Pre-cooked_pasta” including the reflectance spectra collected for each sample. In the Row Labels section are reported 5 class sets:

- i) Sample_ID: identification labels of each block of 50 measurements;
- ii) Dry_weight_content_%: labels of the dry weight content measured on pasta product samples (42.8%, 46.7% and 47.5%);
- iii) Pasta_type_&_phy_con: labels of the pasta product type referring to the physical condition (“Mezze Penne (frozen)”, “Pennette 72 (frozen)”, “Mezze Penne (thawed)” and “Pennette 72 (thawed)”);
- iv) Phy_con: labels of the pasta products physical condition (“Frozen pasta” and “Thawed pasta”);
- v) Pasta_type: labels of the pasta product type (“Pennette 72” and “Mezze Penne”).

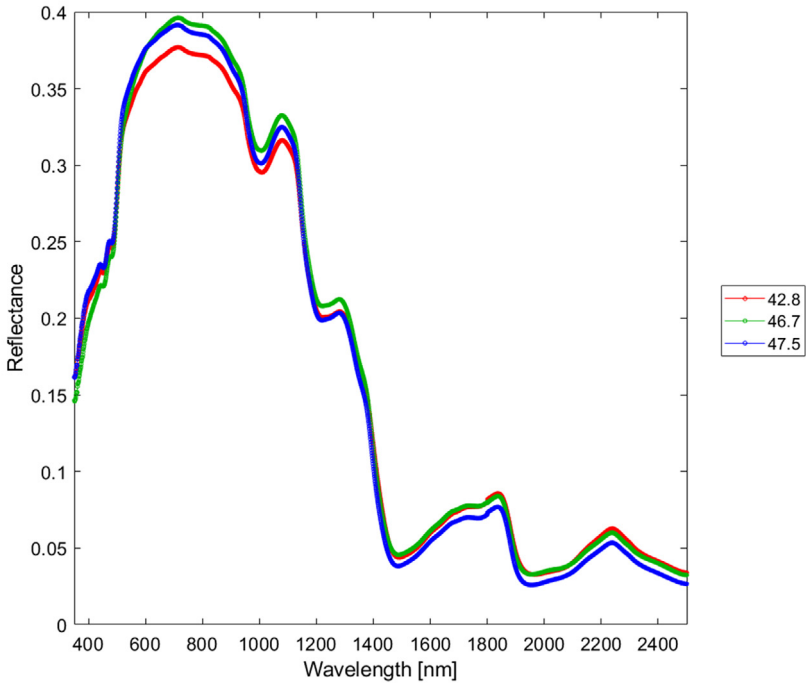
Reflectance spectra according to each class set are reported in Fig. 1. The “Precooked_pasta” DSO size (Number of spectra = 1200) is sufficient to build and validate multivariate models. Data are also provided in .csv format (“Precooked_pasta.csv”). The instrument was calibrated before each set of acquisitions (i.e. after each block of 50 measurements), in order to ensure the repeatability of the acquired data.

The averaged spectra of the pasta products characterized by different salting levels mainly differ in the visible region as can be seen in spectra plots (Fig. 1b and e). While the averaged spectra of the frozen and thawed samples mainly differ in intensities around most of the entire investigated spectral range (Fig. 1c and d). More in detail, “Frozen pasta” spectra show higher reflectance values than “Thawed pasta” in the spectral ranges: 350–1450 nm, 1600–1850 nm, and 2100–2400 nm. Furthermore, the averaged spectra of the frozen pasta products show more pronounced absorbances around 1450–1550 nm and 1900–2100 nm.

The strategy adopted to perform measurements is summarized in Fig. 2. Reflectance spectral data were collected by a portable spectrophotometer, after a specific calibration procedure. Reflectance spectra were then pre-processed to eliminate the “gaps” located between the various acquisition domains of the three detectors of the ASD spectrophotometer. All the gathered information can be imported into MATLAB environment to perform the analysis.



a



b

Fig. 1. Raw reflectance spectra (a) and spectra averaged according to the following class sets: dry weight content (b), pasta product type referring to the physical condition (c), pasta products physical condition (d), and pasta product type (e).

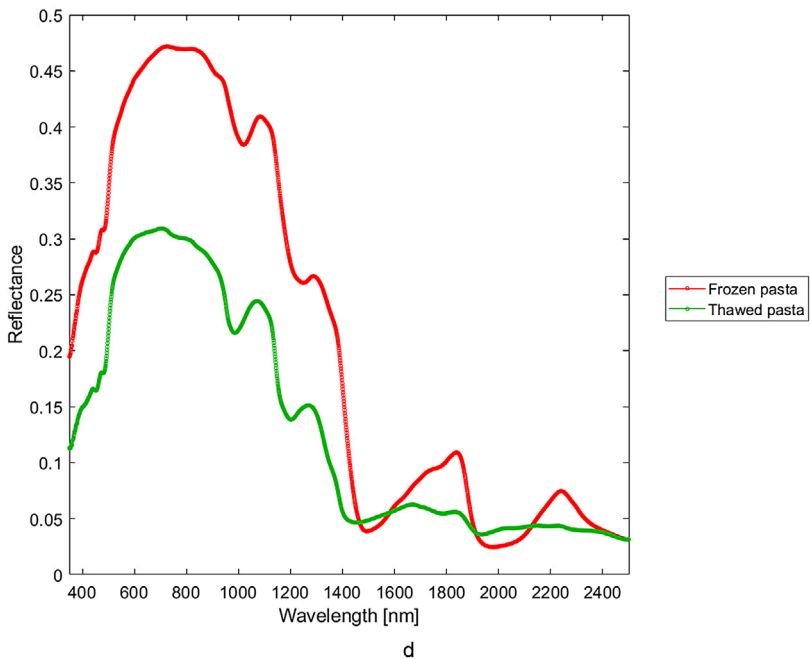
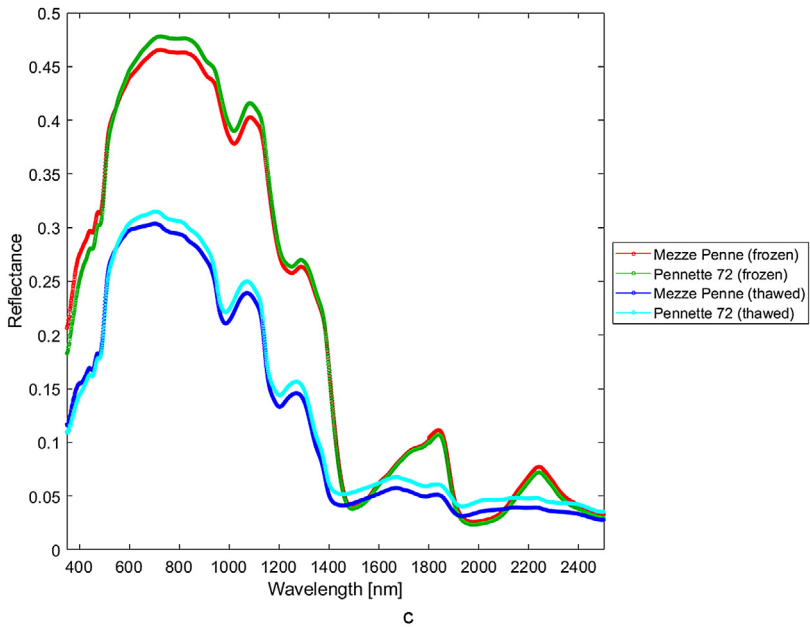


Fig. 1. Continued

2. Experimental Design, Materials and Methods

Samples. The pasta samples analyzed in this study were provided by a company Gelit SpA, located in Cisterna di Latina (Lazio, Italy). The analyzed samples consist of two types of pre-cooked pasta products, with two different degrees of salting: 6 samples of *Pennette72* and 6

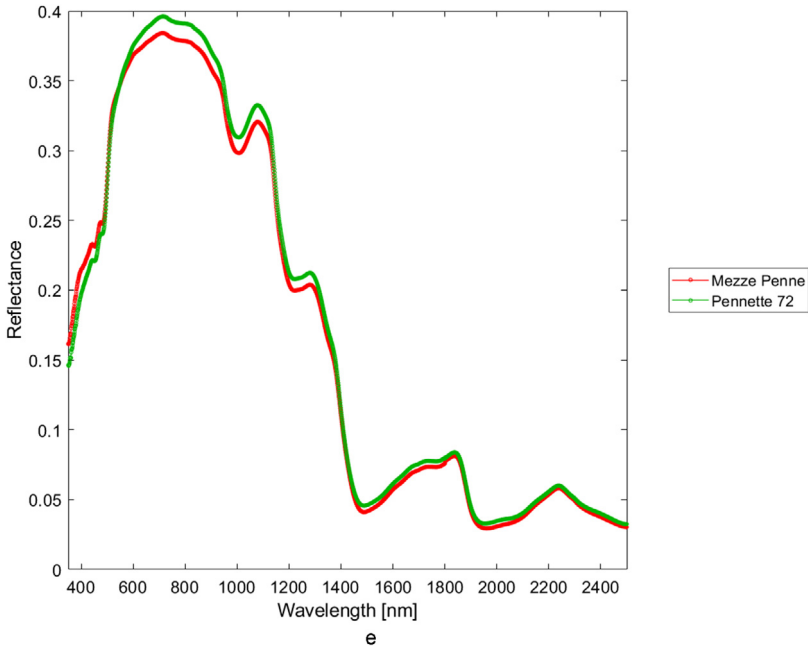


Fig. 1. Continued

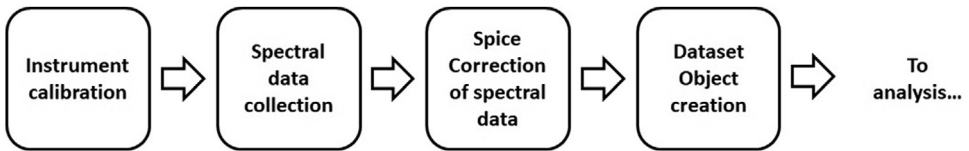


Fig. 2. Schematic drawing of the adopted data handling procedure.

samples of *Mezze Penne*. Approximately 200 g of each sample was placed in different plastic plates. Reflectance spectra were then collected in two stages: frozen (just taken out from the dry ice icebox) and thawed (after about two hours left to rest at a temperature of 26 °C).

Portable spectroradiometer system and spectra acquisition. Vis – SWIR (Visible – Short Wave InfraRed) A portable ASD FieldSpec® 4 Standard–Res spectrophotoradiometer was utilized to collect reflectance spectra.

The spectroradiometer, working in the 350 and 2500 nm wavelength range, is characterized by three detectors characterized by different spectral resolutions: 3 nm at 700 nm and 10 nm at 1400/2100 nm [20]. The instrument, controlled by a portable PC, is constituted by a detectors case and a fiber optics cable connected to a contact probe to perform reflectance measurements.

The spectrophotoradiometer has 3 different holographic diffraction gratings, each one coupled with a detector. In the detector case, order separation filters cover each detector for suppressing second and higher-order light.

Spectra are collected in 3 different wavelength ranges: 350–1000 nm, 1001–1800 nm, and 1801–2500 nm. Detection in the different wavelength ranges is carried out utilizing a 512 silicon array, a first Graded Index InGaAs photodiode (two stages TE cooled), and a second Graded Index InGaAs photodiode (two stages TE cooled) detectors, respectively. The energizing system, embedded in the contact probe, consists of a halogen bulb light source (color temperature equal to 2901 ± 10% °K). The length of the probe, including the grip, is about 25 cm. Inside the probe,

the light source is placed at 12° from the normal axis to the contact probe spot plane (light source angle). The fiber optic head is placed at 35° from the normal axis to the contact probe spot plane (measurement angle). The spot size of the contact probe is 10 mm. The native software RS³ of the ASD instrument was used for data acquisition [20].

Instrument calibration procedure and spectral data handling. ASD FieldSpec[®] 4 Standard-Res spectroradiometer calibration was carried out utilizing a standardized white Spectralon[®] ceramic material from LabSphere, Inc. to set up the “white reference” (W_i). “Dark reference” (D_i), was computed utilizing the dark current calibration file. After this calibration stage, the spectrum is acquired (R_{0i}) and then reflectance (R_i) is computed by the ratio $(R_{0i} - D_i)/(W_i - D_i)$.

The RS3 software (ASD Inc.) was utilized to perform the whole calibration and the spectra acquisition. Collection procedures are reported in “.asd” data files. Instrument “.asd” data files were stacked into an ASCII text file with the aid of ViewSpec Pro (Ver. 6.2.0.) software (ASD Inc.). The “fieldspec_import.m”, available at GitHub [21], was utilized to import the obtained ASCII text file into MATLAB[®] (MATLAB R2016b; Ver. 9.1.0.). Data were stored into a DSO and classes were set by using PLS_toolbox (ver. 8.2.1) by Eigenvector Research Inc.

Spectra acquisition. For each sample, 50 reflectance spectra were acquired by an ASD FieldSpec 4[®] Standard – Res spectrophotoradiometer equipped with a contact probe, in two different times: on frozen and thawed samples (for a total of 600 spectra for frozen samples and 600 spectra for thawed samples). Data acquisition was carried out using the ASD RS3[™] software. The computed grand averages for all subjects of the raw mean spectra are shown in Fig. 1.

Spectra pre-processing. Spectra have been preprocessed in order to reduce noise, minimizing, at the same time, degradation of the essential information. The pre-processing algorithm applied to the spectral data was the so-called Splice Correction (SC) [22]. It was applied to eliminate the “gaps” located between the various acquisition domains of the three detectors of the ASD spectrometer. To make the user free to choose any preferred preprocessing method, the Vis-SWIR spectra included in the present dataset are only preprocessed with SC.

CRediT Author Statement

Giuseppe Bonifazi: Conceptualization, Methodology, Validation, Resources, Writing - Review & Editing, Visualization, Supervision; **Riccardo Gasbarrone:** Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data Curation, Writing - Original Draft, Writing - Review & Editing, Visualization; **Giuseppe Capobianco:** Conceptualization, Validation, Writing - Original Draft, Writing - Review & Editing; **Silvia Serranti:** Conceptualization, Methodology, Validation, Resources, Writing - Review & Editing, Visualization, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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