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Data Article

# A dataset of visible – short wave infrared reflectance spectra collected *in–vivo* on the dorsal and ventral aspect of arms

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ABSTRACT

Advancement of technology and device miniaturization have made near infrared spectroscopy (NIRS) techniques cost–effective, small–sized, simple, and ready to use. We applied NIRS to analyze healthy human muscles in vivo, and we found that this technique produces reliable and reproducible spectral "fingerprints" of individual muscles, that can be successfully discriminated by chemometric predictive models. The dataset presented in this descriptor contains the reflectance spectra acquired in vivo from the ventral and dorsal

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aspects of the arm using an ASD FieldSpec® 4 Standard–Res field portable spectroradiometer (350–2500 nm), the values of the anthropometric variables measured in each subject, and the codes to assist access to the spectral data. The dataset can be used as a reference set of spectral signatures of "biceps" and "triceps" and for the development of automated methods of muscle detection.



## Specifications Table

| | |
|---|---|
| Subject | Spectroscopy. |
| Specific subject area | Biophotonics; clinical application; muscle detection. |
| Type of data | Tables (.csv and .mat files). |
| How data were acquired | Reflectance spectra were acquired in vivo by a portable spectroradiometer from the upper limb muscles. 50 spectra acquisitions for biceps and triceps in each subject, were performed using an ASD FieldSpec® 4 Standard–Res field portable spectroradiometer. |
| Data format | Raw; Analyzed. |
| Parameters for data collection | Normal subjects having no history of skin or musculoskeletal abnormalities involving the upper limb, no abnormality of skin color, no sign of skin disease, no sign of neurological condition other than sporadic episodic headache, no systemic condition, and no regular drug assumption known to induce secondary muscle abnormality. |
| Description of data collection | Spectra were acquired with the muscle at rest, the segment fully supported, and the limb held in fixed posture (elbow angle at 90°), by using a reflectance contact probe. |
| Data source location | Institution: Academic Neurology Unit, A. Fiorini Hospital, Department of Medical–Surgical Sciences and Biotechnologies, Sapienza University of Rome.<br>City/Town/Region: Terracina (LT).<br>Country: Italy. |
| Data accessibility | The datasets described in this paper are hosted in a public repository.<br>Repository name: Bonifazi, Giuseppe; Currà, Antonio; Gasbarrone, Riccardo; Trompetto, Carlo; Fattapposta, Francesco; Pierelli, Francesco; Missori, Paolo; Serranti, Silvia (2020), "A dataset of Visible – Short Wave<br>InfraRed reflectance spectra collected in–vivo on the dorsal and ventral aspect of arms", Mendeley Data, v1.<br>Direct URL to data: http://dx.doi.org/10.17632/24pg3ywxs5.1<br>Instructions for accessing these data:<br>It is not required any access control to data. All study participants provided written consent before being included in the study, which was approved by the institutional review board (Comitato Etico Lazio 2, protocol number 0167183/2018). All methods were carried out following the relevant guidelines and regulations. The stored data does not contain any reference to participants. |
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## Value of the Data

- Datasets can be used as a reference set of spectral signatures of "*biceps*" and "*triceps*" muscles, and for the development of automated methods of muscle detection.

- Life–sciences researchers investigating muscle physiology or disease, engineers and physicists involved in the medical application of photonics, and statisticians expert in chemometric analysis will benefit from these data, on a case–by–case basis, and depending on the personal investigation.
- Data can be used to set up and perform quantitative regressions (e.g. multivariate regression models) and/or classifications (e.g. multivariate classification models).
- Spectral data presented here are the first NIRS fingerprints collected from human muscles in vivo. Therefore, they represent a reference starting point to be replicated and extended. If appropriately implemented as a procedure, muscle spectral fingerprints might be potentially used to refine the diagnostic work–up in primary and secondary muscle diseases, without significant cost and time penalties, thereby improving both clinical practice and investigation.

## 1. Data Description

To perform both qualitative and quantitative analysis of materials, techniques such as optical spectroscopy and related chemometric analysis are increasingly applied. In this scenario, Near Infra–Red Spectroscopy (NIRS) is considered as one of the best analytical tools to perform quality control actions [1,2]. NIRS has been utilized widely to set up a not invasive nor destructive analysis of samples. By using the light they reflect to build characteristic spectra, NIRS provides information on the examined material, that is given as a spectral "fingerprint". Spectra may be used as surrogate markers embedding information on the current status of both organic and inorganic samples. By subjecting their spectra to chemometric analytical tools, samples can be studied, characterized, and classified with no need for classical chemical analysis. At present, NIR spectroscopy is applied for performing systematic environmental remote and proximal sensing [3–6]; in the agri–food industry, where the determination of authenticity and detection of adulteration exerts relentless pressure, the combined application of NIRS-based detection and chemometrics allows to predict chemical constituents in animal meats [7], discriminate fresh or thawed muscles [8], and classify specific muscles from the same animal [9].

Because the classical microscopic studies have revealed that the muscle tissue has specific optical properties, we investigated whether living human muscles might profit from spectral and chemometric analysis [10–12]. We reasoned that having a cheap, reliable, time-sparing, and widely applicable technique for non–invasive in vivo analysis of human muscles could significantly boost both clinical practice and investigation. Therefore, a series of experiments were performed in normal subjects aimed to collect reflectance spectra from the ventral and dorsal sides of the arm, a body segment housing two different muscle groups: flexors (*biceps* and *brachialis*), and extensors (*triceps*). A portable spectroradiometer operating in the 350–2500 nm wavelength range (visible short-wave infrared: Vis–SWIR), was used for collecting spectra. As reported in our previous work, chemometric techniques were applied for exploring data and setting up a model to discriminate muscles [12].

Enrolled participants in the study are 20 Caucasian, southern European healthy subjects (age 25–89 years, 9 women). Their demographic (sex, age), clinical (drugs and/or conditions), and anthropometric data (height, weight, BMI) have been reported elsewhere [12].

The data records presented in this paper are reported in a public repository (i.e. Mendeley Data) and consist of MATLAB (MathWorks Inc., Natick, MA, USA) ".mat" files. More in detail, the "DATASET_matlab.mat" is a MATLAB data file containing two DataSet Objects (DSO):

i) Table – A DSO including the demographic and anthropometric data of study participants (Sex: male=0, female=1);
ii) Reflectance_spectra – A DSO including the Reflectance spectra collected for each subject on each ventral/dorsal aspect of an arm (*D*=dorsal arm; *B*=ventral arm).

Anthropometric data ("Table.csv") and spectral data ("Reflectance_spectra.csv") are also provided in the ".csv" format file.

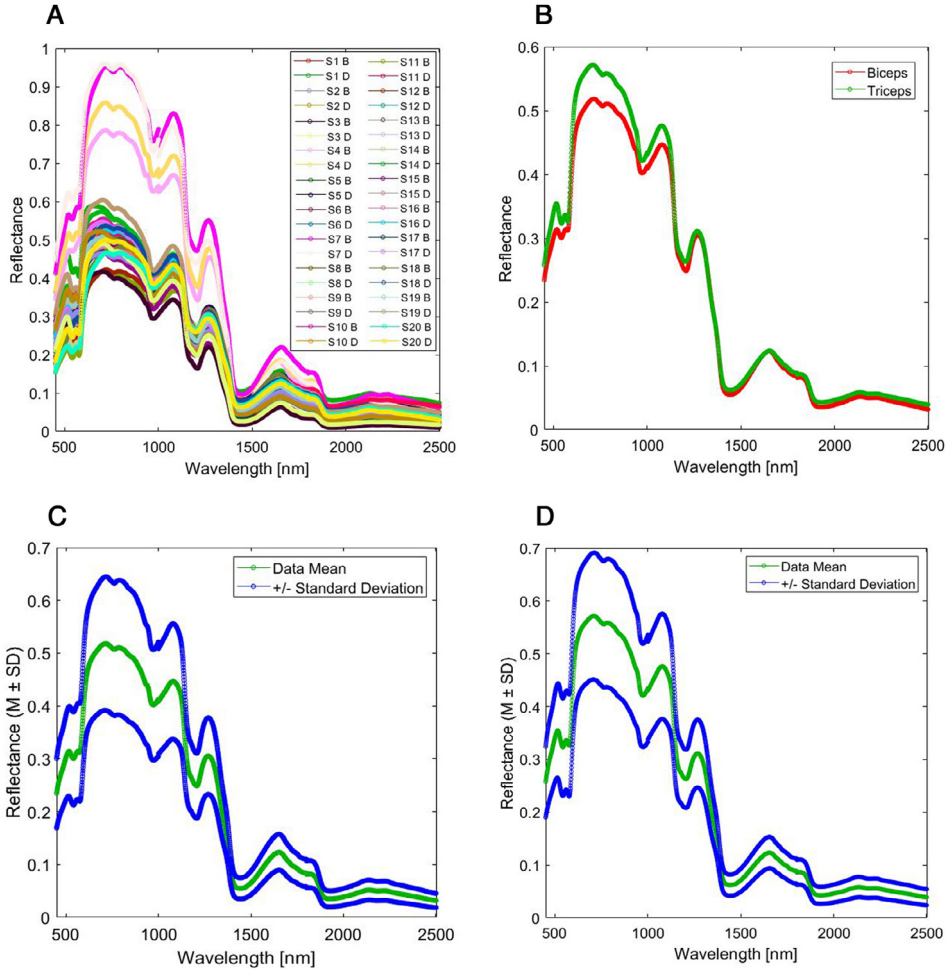


**Fig. 1.** Raw reflectance spectra of *biceps* – B – and *triceps* – D – for each subject (a); grand averages of the reflectance spectra for *biceps* and *triceps* (b); mean and standard deviations for *biceps* (c), and *triceps* reflectance spectra (d).

Reflectance_spectra dataset size (Number of spectra = 2000) is sufficient for constructing and validating multivariate models, e.g., NIRS models. To ensure reproducible NIR measurements, the instrument was calibrated before each set of acquisitions (that is, after each block of 50 measurements). The coefficient of variation (CV) of the spectra acquired on the ventral aspect of an arm ($N = 1000$; class "*Biceps*") is $1.43 \pm 0.57$; the CV of the spectra acquired on the dorsal aspect of an arm ($N = 1000$; class "*Triceps*") is $1.39 \pm 0.61$. Mean reflectance spectra and their standard deviations are shown in Fig. 1c and Fig. 1d.

The shape of the reflectance spectra differentiates the spectra acquired from the ventral and dorsal aspects of the upper arm, around the following wavelengths: 760 nm, 970 nm, 1200 nm, and at 1440 nm (Fig. 1). These wavelengths correspond to reflectance minima determined by specific adsorbing groups and i.e. $H_2O$, CH, $CH_2$ (762 nm); $H_2O$, CH (973 nm); CH (1206 nm); $H_2O$, CH, ROH, $CONH_2$, CONHR (1442 nm); CH (1796 nm); $H_2O$, RCO2R, $CONH_2$ (1930 nm); and $RNH_2$, CHC, CC (2186 nm), that prove able to distinguish the muscles lying under the probe [12]. Indeed, they proved very similar to spectral reflectance minima in meat classification studies [7 – 9]. In addition, in a human study the absorbance peak at 762 nm is "more pronounced in

muscles than in the other tissues" (e.g., the forehead and abdomen), and is attributed to the oxidation of myoglobin (deoxymyoglobin) [12].

## 2. Experimental Design, Materials and Methods

The strategy adopted for performing measurements, and the gathered corresponding data are summarized in Fig. 2. The reflectance spectral data were collected by a portable spectrophotoradiometer and the demographic/anthropometric data were evaluated by administering a survey. All the gathered information could be imported in MATLAB environment as DSO for performing analysis. We adopted different chemometric strategies in order to set up classifiers for distinguishing the spectra collected from the ventral and the dorsal aspect of the arm [12]. The following sections are expanded versions of the description of the devices and methods presented in our previous work [12].

### 2.1. Subjects

Study participants were all normal subjects. They were enrolled among relatives and caregivers of patients coming to the Academic Neurology Unit. Participants were selected according to the following criteria: no history of skin or musculoskeletal abnormalities involving the upper limb, no abnormal color nor other signs of skin disease, no evidence of neurological conditions other than sporadic episodic headache, no systemic condition, no regular assumption of drugs known to induce secondary muscle changes. Hypertension and dyslipidemia were not considered as exclusion criteria.

Following these criteria, 20 Caucasian, southern European healthy subjects (age 25–89 years, 9 women) were recruited.

### 2.2. Portable spectroradiometer system and spectra acquisition

Vis – SWIR (Visible – Short Wave InfraRed) Reflectance spectra were acquired by a portable spectroradiometer from the dorsal and ventral aspect of the upper limb. 50 spectra acquisitions for *biceps* and 50 for *triceps* were performed in each subject by using an ASD FieldSpec® 4 Standard–Res field portable spectroradiometer. Spectra collection was performed with the limb held in a fixed limb posture (elbow angle approximately 90°), by the same operator.

The ASD FieldSpec® 4 Standard–Res portable instrument works in the spectral range 350 – 2500 nm with a spectral resolution of 3 nm at 700 nm and 10 nm at 1400/2100 nm [13]. This portable spectroradiometer essentially consists of a detectors case and a fiber optics cable with

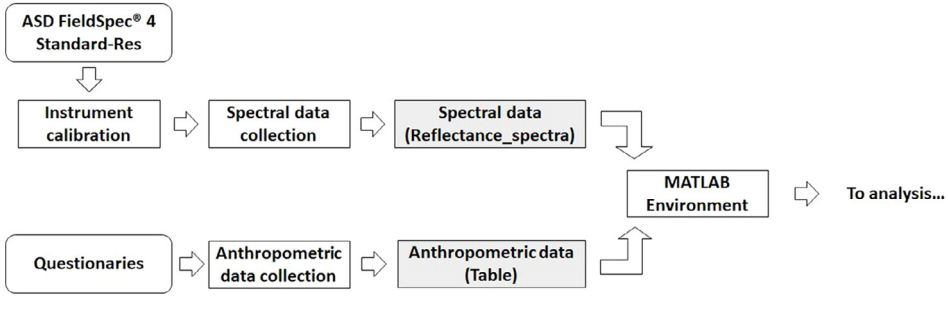


**Fig. 2.** Schematic drawing of employed measurement techniques and the corresponding data.

a contact probe, connected to a personal computer/laptop. Spectrograph architecture consists of 3 different holographic diffraction gratings, each one coupled with a detector. The order separation filters cover each detector for suppressing second and higher–order light. 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 have been utilized to collect spectra in the wavelength ranges 350–1000 nm, 1001–1700 nm, and 1701–2500 nm, respectively.

The ASD Contact Probe consists of a halogen bulb light source with a color temperature equal to $2901 \pm 10\%$ °K. It has a length of 25.4 cm (including the probe grip), and a weight of 0.7 kg. 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 $RS^3$ of the ASD instrument was used for data acquisition [13].

### 2.3. Instrument calibration procedure and spectral data handling

The calibration of the ASD FieldSpec® 4 Standard–Res spectroradiometer was performed by setting a "dark reference" ($D_i$), calculated referencing the dark current calibration file, and by acquiring a "white reference" ($W_i$), measuring a standardized white Spectralon® ceramic material from LabSphere, Inc. After this calibration stage, the spectrum is acquired ($R_{0i}$) and then reflectance is computed according to Eq. (1):

$$R_i = \frac{R_{0i} - D_i}{W_i - D_i} \tag{1}$$

The whole calibration procedure was performed in $RS^3$ software (ASD Inc.). This spectrum collection procedures results in ".asd" data files. Instrument ".asd" data files were stacked into an ASCII text file by the aid of ViewSpec Pro (Ver. 6.2.0.) software (ASD Inc.). The "fieldspec_import.m" [14], a script file specifically written, was utilized to import the obtained ASCII text file into MATLAB® (MATLAB R2016b; Ver. 9.1.0.). Data were stored into datasets objects, and classes were set by using PLS_toolbox (ver. 8.2.1) by Eigenvector Research Inc. The spectral dataset was reduced from 350 to 2500 nm to 450–2500 nm. Since spectral data are likely to include hardware- and/or environment-related noise, spectral preprocessing is required for eliminating noise without degrading essential information. To make the user free to choose any preferred preprocessing method, the Vis–SWIR spectra included in the present dataset underwent no preprocessing.

The MATLAB® script used to import reflectance spectra ".txt" files from ViewSpec Pro, is available at GitHub [14].

### 2.4. In vivo spectra acquisition

The reflectance spectra (350 – 2500 nm) were acquired from the ventral and dorsal aspects of the upper limb by using an ASD FieldSpec® 4 Standard-Res portable spectroradiometer. The same procedure was carried out for collecting all spectra. A health professional placed the instrument contact probe on the subject's limb skin, while an engineer controlled the spectroradiometer from a remote laptop. The contact probe position was standardized according to the locations of motor points. The muscle motor entry point is the position where the motor branch of a nerve enters the muscle belly, and it represents an unequivocal anatomical landmark. Spectra collection was performed for each subject with the muscle at rest, the segment fully supported, and the limb held with an elbow angle at approximately 90° To increase the precision and accuracy of data collection, 50 spectra were acquired from each contact point (50/side/subject, 100 spectra/subject, 2000 spectra in the study). The time required to acquire a single spectrum was around 2 s, thus the entire block acquisition lasted approximately 100 s . Raw reflectance spectra

of the “ventral arm” and “dorsal arm” were collected for each subject (Fig. 1a). The computed grand averages for all subjects of the raw mean spectra are shown in Fig. 1b.

## Ethics Statement

All study participants provided written informed consent before being included in the study. The investigation was approved by the institutional review board (Comitato Etico Lazio 2, protocol number 0167183/2018). All methods were carried out under the relevant guidelines and regulations.

## 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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