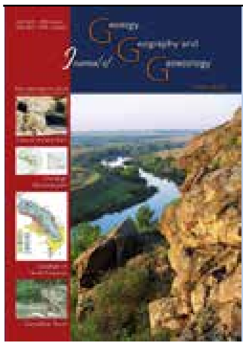

Journal of Geology, Geography and Geoecology

Journal home page: geology-dnu.dp.ua

ISSN 2617-2909 (print)
ISSN 2617-2119 (online)

Journ. Geol. Geograph. Geology, 31(2), 260–272.
doi:10.15421/112224

Use of visual-diagnostic color parameters of soils and optical reflectometry for determination of organic carbon content

Andriy I. Herts[1], Volodymyr O. Khomenchuk[1], Oleksandr B. Kononchuk[1] , Nataliia V. Herts[1], Viktor S. Markiv[1], Andrii O. Buianovskyi[2]

[1]Ternopil National Pedagogical University named after V. Hnatyuk, Ternopil, Ukraine, herts@chem-bio.com.ua
[2]Odesa I.I.Mechnikov National University, Odesa, Ukraine

Received 28.08.2021
Received in revised form 09.09.2021
Accepted 18.09.2021

Abstract. To get additional tools for the assessment of carbon sequestration, along with the visual assessment of soil coloration with the applying of A. H. Munsell's atlas, the analysis of color and spectral characteristics of soil using portable colorimeter NixPro and reflectometer Our Sci Reflectometer was carried out in this study. Elemental analysis of soil samples using X-ray fluorescence analysis was performed and the content of organic carbon was estimated. The spectral range of reflected light, which correlates most with the content of organic soil substance, was singled out. Based on the data, received by methods of reflectometry and colorimetry, prognostic regression models were constructed. A multiple linear regression equation with a statistically authentic luminosity predictor (L*) (R^2=0.61) was obtained. It allows describing the link between the content of the organic substance in the studied soils and the parameters of the color setting system CIELab, as well as the equation describing 69 % of the data link dispersion between the integrated reflection coefficient and the organic carbon content of the soil. The link between the integral reflection coefficient and the total organic substance content was found. The most correlated spectral range with the content of organic substance – 500–632 nm was singled out. Regression models, which were based exclusively on the spectral data of pre-treated H_2O_2 soils, increased their predictability by 8–10 %. Approaches that can complement the tools for rapid determination of the organic carbon content in the soil were presented in the work. Researchers are expanding their arsenal of technical support for estimation of color or spectral coefficients of light reflection, based on which it is possible to conduct geospatial analysis and determine the content of the organic substance in low-humus soils with a probability of 69 %.

Keywords: soil organic carbon, soil color, soil spectral characteristics, regression analysis, NixPro™, Our Sci Reflectometer

Використання візуально-діагностичних колірних параметрів ґрунтів та оптичної рефлектометрії для визначення вмісту органічного Карбону

А. І. Герц[1], В. О. Хоменчук[1], О. Б. Конончук[1], Н. В. Герц[1], В. С. Марків[1], А. О. Буяновський[2]

[1]Тернопільський національний педагогічний університет ім. В. Гнатюка, Тернопіль, Україна, herts@chem-bio.com.ua
[2]Одеський національний університет імені І. І. Мечникова, Одеса, Україна

Анотація. У роботі, з метою отримання додаткового інструментарію для оцінки секвестрації Карбону, поряд з візуальною оцінкою забарвлення ґрунту із застосуванням атласу А. Г. Манселла, здіснено аналіз колірних та спектральних характеристик ґрунту засобами портативного колориметра NixPro та рефлектометра Our Sci Reflectometer. Проведено елементний аналіз зразків ґрунту за допомогою рентгенфлуоресцентного аналізу та оцінено вміст органічного Карбону. Виокремлено спектральний діапазон відбитого світла, який найбільше корелює із вмістом органічної речовини ґрунту. На основі даних, отриманих методами рефлектометрії та колориметрії, побудовано прогностичні регресійні моделі. Отримано рівняння множинної лінійної регресії із статистично достовірним предиктором світлосили (L*) (R^2=0,61), що дозволяє описати взаємозв'язок між вмістом органічної речовини у досліджених ґрунтів та параметрами системи задання кольорів CIELab, а також рівняння, що описує 69 % дисперсії даних взаємозв'язку між інтегральним коефіцієнтом відбиття та вмістом органічного Карбону ґрунту. **Виявлено**, **взаємозв'язок** між інтегральним коефіцієнтом відбиття та загальним вмістом органічної речовини. Виокремлено найбільш скорельований із вмістом органічної речовини спектральний діапазон – 500–632 нм. Регресійні моделі, які базувались виключно на спектральних даних попередньо оброблених H_2O_2 ґрунтів, підвищували свою прогностичність на 8–10 %. В роботі представлено підходи здатні доповнити інструментарій експрес визначення вмісту органічного Карбону у ґрунті. У дослідників розширюється арсенал технічного забезпечення для оцінки колірних чи спектральних коефіцієнтів відбиття світла, на основі яких можна проводити геопросторовий аналіз і здійснювати, з ймовірністю 69 %, визначення вмісту органічної речовини у слабо- і малогумусних ґрунтах.

Ключові слова: ґрунтова органічна речовина, органічний Карбон, колір ґрунту, спектри відбиття, регресійний аналіз, NixPro™, Our Sci Reflectometer

Introduction

Carbon is one of the main components of soil organic matter (SOM), which largely determines soil fertility (Fu et al., 2020). Preservation and restoration of soil humus as the main storage of carbon, as well as nitrogen, phosphorus, sulfur and other plant nutrients is a necessary condition for sustainable agriculture (Fu et al, 2020). Information that characterizes the amount of organic matter in the soil becomes a decision-making tool not only in agriculture, but also is crucial in mitigating the global effects of climate change, etc. (Lorenz and Lal, 2014).

Currently, the issue of introduction of new highly informative criteria for assessing the condition of the soil cover, in particular the amount of organic carbon, is relevant. Since the classical methods of organic matter analysis in representative landscape soil samples are very long and laborious, today research is being done for rapid methods for assessing the processes occurring in the soil, especially the dynamics of carbon content (Mikhailova et al, 2017; Swetha and Chakraborty, 2021).

Given the fact that organic matter is one of the main components that determine the color of the upper horizons of most types of soils, the assessment of its content by color, spectral characteristics, is a promising method of research (Karavanova, 2003). The fact that the patterns of light reflection by soils are quite complex and depend on the chemical composition, properties and structure of the soil, does not reduce the efficiency and feasibility of using its spectral characteristics as a criterion (de Santana FB et al, 2018).

In view of this, a promising approach in the study of soil properties is the study of color and spectral properties using technical means that exclude the subjective factor. Thus, in the works of a number of authors (Karavanova and Orlov, 1996; Moritsuka et al., 2014), the analysis of soil parameters was carried out through the color parameters of the soil, which were obtained using colorimeters. Thanks to the readers of the color characteristics of the soil, the researchers obtain the values L (lightness), a (redness), b (yellowness) of the color system CIEL* a* b* (CIELab) and perform a rapid assessment of the total content of C, N and Fe in agricultural soils (Moritsuka et al., 2014). In (Fu et al., 2020), the potential of digital cameras, including smartphone cameras (Fan et al., 2017), in measuring soil color was demonstrated. A number of researchers (Stiglitz et al, 2015; Stiglitz et al, 2017; Moritsuka et al, 2019; Mukhopadhyay and Chakraborty, 2020) in their works describe the possibilities of inexpensive colorimeters, such as Cube (Moritsuka et al, 2019), NixPro (Mukhopadhyay and Chakraborty, 2020; Swetha and Chakraborty, 2021), Color Muse (Moritsuka et al, 2019), which allow non-specialists, such as farmers, gardeners and students, to measure soil color with instruments, to study the relationship between color characteristics and component composition of the last one, and to use the data obtained for the classification of soil differences, etc.

In contrast to the above-mentioned instruments, the information of which comes in the form of values of color models CIELab, RGB, Munsell et al., spectrophotometers and reflectometers are being widely used in the study of soils. The work of the latter is based on the idea of using the spectral reflectivity of the soil in the visible and IR parts of the spectrum, where a special role in the formation of these characteristics is played by organic matter (Kawamura et al, 2017; Marques et al, 2019).

This paper presents an approach that allows, using a portable colorimeter NixPro™ and Our Sci Reflectometer (Ewing et al, 2021), to obtain color characteristics, spectral curves of reflection of radiation, to calculate spectral and integral coefficients of light reflection of different soil types, to identify spectral ranges most correlated with organic carbon content in the studied soil samples. This will allow to check the effectiveness of this type of devices for express assessment of the content of organic matter in the soils of the region.

Materials and methods

The soil for the study was selected from the territory of Ternopil, Lviv and Ivano-Frankivsk regions in 2019. A total of 17 geographically separated areas were covered (Table 1). Sampling was carried out according to the standard method from agricultural lands. Soils were classified according to the Predicted World Reference Base (WRB) (FAO of the United Nations, 2015). The main physicochemical parameters (Table 1) were obtained according to the GPS coordinates of soil selection and using the SoilGrids REST API in RStudio and Phyton.

To determine the color and measure the reflection spectra, the soil was air-dried and sieved through a sieve with a hole diameter of 1 mm to obtain a more homogeneous mixture of structural aggregates, the size of which is known to affect soil reflectivity (Karavanova, 2003).

A. G. Munsell's universal optical system was used to assess visually the color of the soil (Munsell Color, 2018). Soil color was characterized by color hue (Hue, H), lightness or brightness (Value, V) and color saturation (Chroma, C).

The Our Sci Reflectometer was used to measure reflection spectra at ten wavelengths (365 nm, 385 nm, 450 nm, 500 nm, 530 nm, 587 nm, 632 nm, 850 nm, 880 nm, 940 nm) (Ewing PM et al, 2021). To do this, 5 g of soil was placed in a measuring container with a diameter of 30 × 10 mm, which is included in the set of the device. The obtained spectral curves were characterized by such parameters as integral light reflection (ρ_ε) (Karavanova & Orlov, 1996) and spectral reflection coefficients (ρ_λ) (Karavanova & Orlov, 1996) for these ten wavelengths.

In parallel, the color of the soil in the color spaces CIELab, CMYK, RGB was evaluated using a color scanner Nix Pro™ (Hamilton, Ontario, Canada). The samples were placed in the same measuring container as for the study of spectral properties, forming a layer with a thickness of approximately 7 mm. The sensor was placed above, which made it impossible for light to enter from the outside. Nix Pro™ 2 ° / D 50 LED mode.

The content of trace elements (TEs) in the initial soil was determined using the X-ray fluorescence analysis (Pidlisnyuk, V.V. et al, 2020). The results are presented in the Table 2. The content of TEs in the initial soil was typical for such sort of soil and did not violate the standards of EU and Ukraine (Pidlisnyuk, V. et al, 2021).

Oxidation of organic substance in the research samples was performed with hydrogen peroxide. 5 grams of soil, which had been pre-ground and sifted through a 1 mm sieve, had been placed in a porcelain cup. 5, 10, 15, and 20 ml of concentrated H_2O_2 were added in small portions during mixing. After that, the soil was dried, ground, and sieved through a sieve, the reflection spectra were taken, and the carbon content was determined.

Evaluation of soil organic carbon (SOC) was performed by an oxidimetric method based on the oxidation of organic matter of soils and rocks with a solution of potassium dichromate in sulfuric acid, followed by determination of organic carbon content by establishing the residue of potassium dichromate by titrometry method (Pidlisnyuk, V. et al, 2021).

After the research, the mass fraction of carbon (C) of organic matter as a percentage of the the soil mass was calculated according to the formula:

$$C = \frac{(a\text{-}b)\cdot н_1 \cdot 0{,}0003\cdot 100}{P\cdot н_0}, \tag{1}$$

where:

C is the carbon content,%; **a** is the amount of Mora salt solution spent on the titration of the blank, cm^3; **b** is the amount of Mora salt solution spent on titration of the chromium mixture of the sample, cm^3; **$н_1$** is the normality of the working solution of Mora salt; **$н_0$** is the normality of the exact solution of Mora salt 0.1 g-eq / dm^3; **0.0003** is the gram equivalent of carbon, corresponding to 1 cm^3 of Mora salt solution, g/cm^3; **P** is the weight of the soils sample, g; **100** is the conversion factor,%.

Computer processing of the research results was performed in the RStudio environment using the following packages: ggally, corrplot, clusterSim and factoextra (The R Project, 2021).

Regression analysis was used to build a model for predicting the content of SOC. 80 % of randomly selected soil samples were used as a training data set. The remaining 20 % is a test kit that was used for cross-validation and model validation. Soil organic carbon in the multiple linear regression equation acted as adependent variable. Color and spectral characteristics of soil acted as independent variables. Principal component analysis (PCA) was used to reduce the dimensionality and identify relationships between variables. The analysis was performed in an RStudio using the FactoMineR library (The R Project, 2021).

The critical level of significance when testing statistical hypotheses in the study was taken equal to 0.05.

Results

The soils of the studied areas, according to the classification of the Predicted World Reference Base (FAO & IUSS, 2015) belong to the soil groups of Phaeozems and Chernozems. Among the soil units, Haplic soils predominated, which have a typical expression of certain characteristics (Polchina, 2007).

Among the selected samples, according to SoilGrig (Table 1), there were also such soils as: Haplic Fluvisols, Haplic Albeluvisols, Haplic Cambisols, and Luvic Phaeozems.

In its vast majority, according to Munsell, the color tone of the soils of the study area is characterized as 2.5Y and 10YR, that is, yellow and yellow-red, respectively. The studied samples (Table 1) can be characterized as light brown, grayish brown, light olive brown, olive brown, yellowish-brown, dark brown, dark grayish brown, very dark grayish brown, gray, and very dark gray.

The parameters of the CIEL* a* b* color setting system of the investigated soil samples obtained with the help of Nix Pro™ are presented in the Table 1.

In the literature (Stiglitz et al., 2017) there are data describing the potential of NixPro in predicting SOC and total nitrogen in the soil. As in the above-mentioned researchers, one of the statistically significant predictors of our multiple regression equation, which describes the relationship between SOC and CIEL* a* b* color parameters, is L * (Table 4) ($R^2 = 0.61$).

The data obtained are fully consistent with the results of other researchers. In (Swetha & Chakraborty, 2021), the prediction of SOC by color parameters obtained by the Nix sensor (in color models RGB, XYZ and CMYK) was characterized by R^2 at the level of 0.66.

The color change of the soil after its treatment with H_2O_2 is due to the oxidation of organic substances

(Table 2, 3). After the interaction of the studied soil samples with hydrogen peroxide, unlike on the trace elements, parameters of Value and Chroma changed, and as a result, the visual perception of color by the researcher changed too (Table 3). For example, the soil sample No14, which can be described in the Munsell system as 10YR 3/2 (very dark grayish brown), after interaction with 5 ml of H_2O_2 changed color to 10YR 4/1 (dark gray); and under the influence of 10 and 20 ml of hydrogen peroxide it changed to 10YR 4/2 (dark grayish brown) and 10YR 5/2 (grayish brown), respectively.

Using SOC as a dependent variable and L*, a*, b*, as independent ones, we obtain the equation with one statistically significant ($p < 0.001$) predictor L* and the coefficient of determination $R^2 = 0.78$ (Table 4a).

Thus, the action of hydrogen peroxide mainly modulates the two color parameters of the Munsell system – brightness (V), saturation (C), and L*, b* of the color model CIEL*a*b*.

Using the OurSci Reflectometer, the spectral reflection and absorption of light by the soil at wavelengths of 365, 385, 450, 500, 530, 587, 632, 850, 880, 940 nm were estimated. The integrated reflection coefficient ρ_ε (Reflection) of the studied soils has been calculated (Table 1).

The linear regression equation, where the dependent variable is SOC and the independent one is Reflection, describes 69 % of the data variance ($R^2 = 0.69$) (Table 5), which is consistent with other data (Ewing PM et al, 2021). Soil after its treatment with H_2O_2 R^2=0.79.

To identify the relationships between all variables and to visualize quantitative variables, the PCA was used, where the input values were the spectral regions of reflection (365, 385, 450, 500, 530, 587, 632, 850, 880, 940 nm), the integrated reflection coefficient (Reflection) and SOC in a particular soil sample (Corg, fig. 1, 2). This approach allowed to reduce the dimensionality of the data and to find the part of the spectrum which is the most correlated with the content of organic matter, which was 500, 530, 587 and 632 nm in untreated (native) soil and the soil treated with hydrogen peroxide (Fig. 1, 2).

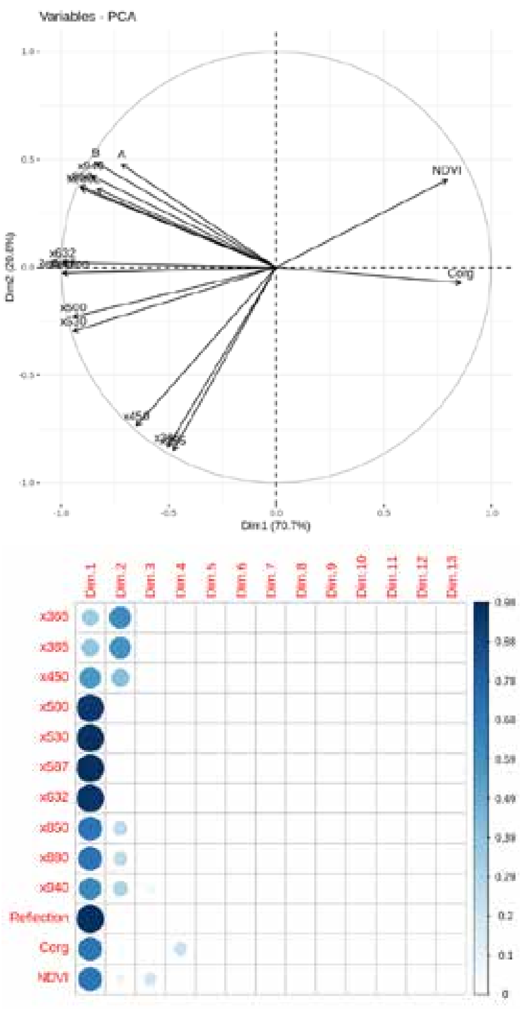

Fig. 1. PCA analyses. Correlation measured spectral soil parameters with the main components

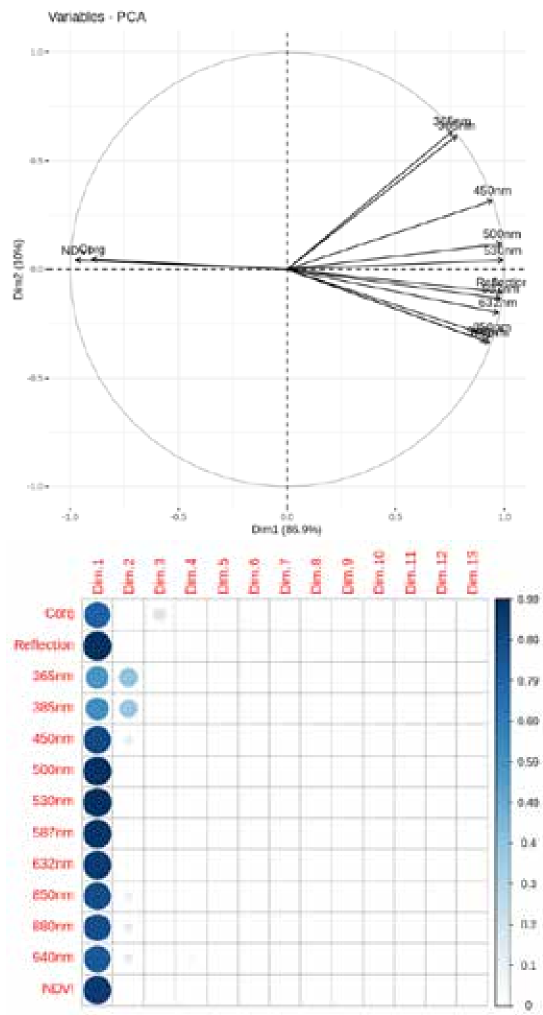

Fig. 2. PCA analyses. Correlation measured spectral soil parameters with the main component for soil treated with hydrogen peroxide

The analysis of the results showed that the first main component (Factor 1) includes 70.7 % of the total data variation (Fig. 1). The second main component (Factor 2) covers 20.8 % of the variance. The largest contribution to the first component (Fig. 1a) is made by the following output variables: Reflection, reflection spectra 500–632 nm and NDVI index (Normalized Difference Vegetation Index).

In the case of the application of PCA to a sample of soils whose organic matter was artificially oxidized by hydrogen peroxide, the first two main components include 96 % of the initial output data (Fig. 2).

Therefore, due to the fact that the studied reflection spectra have different sensitivity to the components of the soil, they contribute differently to the formation of the main components. Figures 1 and 2 show that by including of only the first component in the calculation we can describe with one variable, respectively, 70 % and 96 % of the twelve spectral characteristics of the soil. Using the newly created factors to build a model of linear regression, we obtained equations with coefficients of determination $R^2 = 0.72$ and $R^2 = 0.80$ (Table 5).

Discussion

Currently, the soil color is used as one of the key morphological parameters of horizon differentiation and their classification by types. Soil color underlies the classification of soils by the US Soil Taxonomy (Baillie, 2006) and the World Reference Base (FAO & IUSS, 2015).

In the field conditions, soil color measurement is often performed by visual comparing soil samples with standard color diagrams and tables based on the system presented by the soil scientist T. Munsell. Currently, the table of the soil color by the Munsell Color Company (MSCC) is the main system for determining soil color (Munsell Color, 2018).

Although the researchers (Wills, 2007) in situ conditions showed the existence of a negative correlation between the content of organic matter in the soil and the value of HVC (Hue, H; Value, V; Chroma, C) of Munsell's atlas, an important disadvantage of this technique is its complicated mathematical interpretation (Marques et al., 2019). Obviously, in statistical calculations based on empirical approaches, there will be low accuracy due to the psychophysical and physiological characteristics of the researcher, who will determine the colors (Marques et al., 2019).

In order to avoid subjectivity in the assessment of soil color and to increase the accuracy of measurements, researchers use the technology of color sensors. It significantly speeds up the process and allows you to simultaneously obtain the parameters that characterize the color of the soil of a number of color models: RGB (red, green, blue), XYZ (three-component color space of stimuli), CMYK (blue, magenta, yellow, black), etc.

For soil scientists, the CIELab system is convenient in that the value of L* is inversely related to the content of dark humus pigment in the soil. The value of a* is directly proportional to the content of red hematite pigment αFe_2O_3 in the soil. The value of b* is directly proportional to the content in the soil of the yellow pigment of goethite αFeOON (Stiglitz et al., 2016; Vodyanitskii & Savichev, 2017).

Nowadays, with the help of modern algorithms, it is possible to convert the color coordinates of the Munsell system into the CIEL* a* b* system. The last one is widely used to characterize the color of soils during spectrometric analysis in the laboratory, as well as to assess the contribution of pigments to the color. The procedure of the transformation itself is described in the works of a number of authors (Kirillova et al., 2018).

The use of the multiple linear regression equations allows to describe the relationship between the organic matter content of the studied soils and the parameters of the CIELab color setting system, which were obtained using a portable sensor NixPro.

In (Swetha & Chakraborty, 2021), a number of approaches to improving the accuracy of SOC forecasting are presented. All of them are based on the involved additional tools, and, therefore, a combination of data was obtained from several portable devices. Ultimately, this improves prognostic models. Nowadays, X-ray fluorescence spectrophotometry (XRF) and diffuse reflection spectra are being increasingly used in soil analysis. Morgan et al. (Morgan et al., 2009) used the last ones for the forecast of SOC in their works. The combined use of XRF and NixPro, described in a number of works (Morgan et al., 2009; Kagiliery et al., 2019; Mukhopadhyay et al., 2020), makes it possible to obtain a model with an accuracy of $R^2 = 0.81$. In general, the authors conclude that NixPro in combination with additional soil predictors – texture, clay content, etc., is a fairly reliable tool in addressing the above issues (Zhu et al., 2011; Swetha R. K. & Chakraborty, 2021).

Presently, there are a number of works (Aitkenhead et al, 2018; Mouazen et al, 2007) where spectroscopy in the visible and near-infrared regions of the spectrum was used to analyze the relationships between soil organic matter content and reflection spectra.

Given that NixPro covers only the visible spectral range, the use of a Our Sci Reflectometer, which, according to its technical characteristics (Our-Sci Web Aplication, 2021) operates in a wider spectral range, is appropriate. The efficiency of this reflectometer for predicting the content of SOC has been shown previously (Ewing PM et al, 2021). The accuracy of the forecast based on Our Sci increased, as in the case with NixPro, with the addition of such extra predictors as soil texture, sand, clay, etc.

Thus, based on the integrated light reflection coefficient, the linear regression equation can describe the correlation between soil organic matter and its spectral characteristics.

It should be noted that humic acids of different soil types are characterized by different percentages of carbon and the degree of dispersion, which can make some adjustments to our reflection spectra and create additional statistical error (Karavanova, 2003).

It is known that in different parts of the spectrum the amount of absorbed and reflected light differs, so it is more correct to use the integrated reflection index. According to the literature data, the highest absorption of humic substances is observed in the region of 750 nm (Orlov et al., 2001), so was made success attempt and isolated the spectral range that will most correlate with the content of organic carbon in the studied soils.

The two devices NixPro and Our Sci Reflectometer that were used, showed similar results, which looks quite natural, because, as mentioned above, they work in almost the same spectral range. The proposed approach to constructing equations describing the relationship between SOC and spectral (color) characteristics of the soil, using the main components as independent variables can increase their prognostic accuracy and minimize multicollinearity in regression analysis.

Conclusion

Based on the obtained data, it should be noted that the use of quantitative and qualitative characteristics of light reflected from the soil surface allows to-intact effectively with a high level of reliability and sensitivity to determine the approximate mass fraction of carbon in the soil organic matter.

OurSci and Nix ProTM devices, used to develop SOC forecasting models in the region's soils and controlled by a mobile application via Bluetooth, have shown good results and, therefore, have prospects for further use for these purposes. This type of technology is a reliable and inexpensive means of data collection in the field and laboratory conditions. Special mention should be made of Our Sci Reflectometer as a tool developed in accordance with the principles of «Open Hardware», integrated with the cloud platform OurSci Web Application (Our-Sci Web Aplication, 2021). The last one allows the experimenter not only to export and statistically process the results, but also to visualize the data using on-line platforms, create their own research protocols and make the necessary changes to the algorithms of the device. An unambiguous advantage is that the documentation on the operation of the reflectometer is publicly available, its main technical characteristics are described, the stages of creating protocols (instructions) for device control are described, and so on.

As a result, researchers are expanding the arsenal of technical support, thanks to which it is possible to conduct geospatial analysis, to assess the amount of soil organic matter not only in the laboratory but also in the field.

Taking into account the fact that preliminary (before analysis) H_2O_2 soil treatment allows to obtain 8–10 % more accurate SOC prediction models, we assume that the use of such an additional stage in sample preparation, especially in the laboratory, may be justified. However, further research involving soils from different soil and climatic regions is still needed.

Given that in the studied soils the carbon content in the organic matter varied in a narrow range (0.8–3 %), the coefficient of light reflection from the surface can be a successful tool for rapid assessment of organic carbon content, and hence organic matter in soil with high probability – more than 70 %.

Acknowledgements

The authors are thankful to Greg Austic (Our Sci LCC member/owner) for technical assistance and new opportunities and Our-Sci team for their cooperation, and to Pavlo Shapoval, National University «Lvivska Polytechnika», Ukraine, for providing chemical analysis of initial soil.

Table 1. Characteristics of soils of the studied areas

Soil sample No	Place of selection		Soil classification according to the Predicted World Reference Base	Soil organic carbon content (SOC), %	CIEL*a*b*			Munsell HVC	Integral light reflection ρ_ε, Reflection
	GPS Latitude	GPS Longitude			L*	a*	b*		
1	49.3927099	25.622718	Phaeozems	2.06	39.94	5.15	11.60	10YR 4/2	177.05
2	49.8062357	24.8909885	Chernozems	2.27	37.12	3.56	6.096	10YR 3/1	129.28
3	48.9379293	25.1746257	Luvisols	1.31	48.98	6.913	16.55	2.5Y 5/3	215.98
4	49.1874657	25.7687652	Chernozems	1.65	45.67	4.62	12.35	2.5Y 4/2	179.27
5	49.489446	25.4871618	Chernozems	1.02	43.72	5.84	12.92	10YR 4/2	177.04
6	48.8531533	25.8114637	Phaeozems	1.81	39.52	4.80	11.23	10YR 3/2	151.25
7	49.0615922	25.0144102	Phaeozems	1.0	53.42	5.97	15.78	2.5Y 5/3	219.41
8	49.5889481	25.1716947	Phaeozems	1.82	44.81	5.29	11.86	2.5Y 4/2	146.36
9	49.5390535	24.5235939	Cambisols	1.72	42.49	4.96	11.46	10YR 4/2	128.39
10	49.2039047	26.0909422	Phaeozems	1.41	46.83	5.81	13.97	2.5Y 4/3	171.44
11	49.5594162	25.5048733	Phaeozems	1.98	40.17	5.45	12.17	2.5Y 3/2	130.04
12	50.1568262	23.4478371	Cambisols	1.91	42.29	4.68	10.14	2.5Y 4/2	132.08
13	49.3564161	24.7604685	Chernozems	1.40	49.05	5.46	14.46	10YR 3/2	175.49
14	49.3786846	26.0271247	Phaeozems	2.51	38.12	4.72	9.19	10YR 3/2	129.33
15	49.2095662	25.9000033	Phaeozems	2.40	39.37	4.92	10.50	2.5Y 3/2	138.28
16	49.0764702	26.1660861	Chernozems	1.28	43.83	4.69	12.9	2.5Y 4/2	171.04
17	49.1567037	25.99764	Phaeozems	2.16	43.75	4.62	10.83	2.5Y 5/2	143.91
18	49.2480082	24.9656369	Cambisols	1.12	51.41	7.41	19.14	10YR 5/4	187.06
19	49.6369746	25.1614127	Phaeozems	1.98	39.07	5.39	11.49	10YR 4/2	128.98
20	50.217551	24.8309249	Phaeozems	1.81	42.83	4.093	8.42	10YR 5/1	128.17

Table 2. Elemental analysis of the soils treated and untreated with H_2O_2 (random examples)

TE's µg/kg	Examples													
	2	2*	3	3*	5	5*	7	7*	14	14*	15	15*	19	19*
	-	H_20_2	-	H_20_2	-	H_20_2	-	H_20_2	-	H_20_2	-	H_20_2	-	H_20_2
Mg	4075.26 ± 1241.90	5907.59 ±1148.31	9045.79 ± 947.60	9929.36 ± 935.05	9312.32 ± 936.71	9131.77 ± 931.21	8790.84 ± 926.40	8936.29 ± 931.79	10458.02 ± 1039.71	10504.26 ± 1025.38	8948.58 ± 997.25	10004.46 ± 986.15	8966.23 ± 955.95	8475.28 ± 918.93
Al	50450.23 ± 727.31	47892.36 ± 695.58	62506.51 ± 619.01	65533.68 ± 617.75	61951.42 ± 615.44	62315.55 ± 617.48	61018.01 ± 617.70	63244.43 ± 618.00	59150.57 ± 654.26	59039.76 ± 647.29	64064.69 ± 644.39	66564.68 ± 641.45	63768.31 ± 628.25	59604.42 ± 614.39
Si	283699.51 ± 1010.90	299754.68 ± 1025.51	363497.80 ± 813.13	360118.55 ± 796.90	365383.18 ± 803.35	365073.07 ± 808.81	365874.17 ± 809.92	363927.98 ± 797.10	335105.62 ± 897.70	338989.76 ± 882.98	354781.16 ± 848.45	352992.33 ± 821.18	361166.94 ± 834.13	368855.25 ± 813.10
P	11692.33 ± 517.82	12448.17 ± 502.86	2525.06 ± 360.98	2811.42 ± 358.86	1002.62 ± 355.54	1271.69 ± 361.62	1719.40 ± 366.91	2399.29 ± 359.09	10355.16 ± 427.65	10938.10 ± 432.06	1563.32 ± 377.56	2306.74 ± 364.19	837.62 ± 365.10	479.17 ± 367.09
S	599.15 ± 42.36	456.19 ± 39.51	180.33 ± 28.66	78.37 ± 27.60	139.38 ± 28.03	88.42 ± 27.69	191.44 ± 28.44	104.97 ± 28.36	301.10 ± 31.95	215.65 ± 31.75	280.28 ± 29.89	166.88 ± 29.76	170.68 ± 29.23	131.79 ± 27.69
K	15781.77 ± 1861.52	16036.74 ± 1888.46	23280.09 ± 1740.13	22947.47 ± 1687.87	22620.91 ± 1687.72	22604.06 ± 1652.38	22718.34 ± 1721.32	22097.89 ± 1686.08	25904.05 ± 1681.42	24575.58 ± 1613.58	24932.68 ± 1727.89	23261.87 ± 1677.09	23754.90 ± 1762.86	22216.59 ± 1704.79
Ca	144589.00 ± 1416.11	126612.24 ± 1400.22	7850.54 ± 894.70	6894.49 ± 855.77	8989.37 ± 855.58	8159.76 ± 870.30	8394.44 ± 889.78	7677.62 ± 852.85	35924.28 ± 1030.48	31375.12 ± 999.15	13205.46 ± 937.15	12519.82 ± 889.08	10232.14 ± 915.31	8060.45 ± 872.19
Ti	5642.65 ± 387.05	3722.18 ± 356.78	5165.58 ± 262.60	5627.08 ± 260.39	5341.91 ± 258.40	5559.81 ± 260.36	5875.17 ± 268.32	6225.96 ± 265.94	5373.18 ± 279.13	5428.67 ± 268.88	5895.05 ± 275.71	5504.82 ± 265.99	5622.73 ± 275.73	5760.96 ± 262.41
Cr	127.71 ± 95.20	60.25 ± 93.26	97.34 ± 64.61	112.99 ± 61.13	114.18 ± 62.31	105.15 ± 61.64	76.71 ± 63.12	119.58 ± 61.80	127.72 ± 68.05	117.44 ± 64.38	108.86 ± 66.74	96.03 ± 64.32	74.21 ± 67.21	124.61 ± 62.95
Mn	962.12 ± 70.7	731.93 ± 64.35	867.45 ± 50.26	768.56 ± 46.76	608.15 ± 45.84	626.65 ± 45.57	861.45 ± 48.87	755.91 ± 47.88	859.51 ± 51.61	763.36 ± 50.42	752.02 ± 50.78	763.90 ± 48.95	624.47 ± 48.61	542.67 ± 46.07
Fe	20982.27 ± 172.25	17440.18 ± 153.10	23203.24 ± 138.55	23572.55 ± 135.94	22730.28 ± 132.77	23084.43 ± 136.50	22225.87 ± 133.09	21912.60 ± 131.93	25801.91 ± 154.64	24854.74 ± 149.13	28312.32 ± 157.32	27920.52± 152.49	24729.39 ± 144.61	23224.94 ± 136.58
Ni	26.31 ± 17.79	27.56 ± 16.27	20.52 ± 13.09	30.59 ± 12.33	16.93 ± 12.82	24.85 ± 12.07	25.35 ± 12.76	22.58 ± 12.16	34.33 ± 13.75	28.77 ± 12.74	43.16 ± 13.70	30.03 ± 13.05	24.94 ± 13.54	23.70 ± 12.16
Cu	24.65 ± 11.61	19.11 ± 10.60	17.33 ± 8.19	21.40 ± 7.80	21.59 ± 7.52	19.00 ± 7.57	22.13 ± 7.99	17.19 ± 7.76	29.98 ± 8.82	28.47 ± 8.08	38.13 ± 8.56	32.65 ± 8.31	17.21 ± 8.33	17.51 ± 7.67
Zn	126.34 ± 10.06	101.56 ± 8.98	75.77 ± 6.48	73.06 ± 6.29	52.29 ± 5.82	53.62 ± 5.79	83.37 ± 6.43	81.77 ± 6.40	135.57 ± 7.65	125.48 ± 7.22	82.27 ± 6.87	77.11 ± 6.58	57.20 ± 6.44	54.70 ± 5.97
Sr	95.26 ± 2.97	71.51 ± 2.59	103.86 ± 2.23	104.28 ± 2.17	107.88 ± 2.18	107.50 ± 2.19	109.77 ± 2.22	103.31 ± 2.16	115.09 ± 2.46	107.54 ± 2.35	121.42 ± 2.46	114.89 ± 2.33	111.49 ± 2.34	106.61 ± 2.19
Zr	378.29 ± 4.98	268.78 ± 4.08	97.46 ± 2.17	95.99 ± 2.09	111.23 ± 2.19	110.48 ± 2.24	108.87 ± 2.21	99.55 ± 2.13	149.89 ± 2.68	139.80 ± 2.54	124.18 ± 2.45	122.40 ± 2.37	113.72 ± 2.35	108.91 ± 2.23
Sn	464.90 ± 5.86	148.61 ± 3.93	590.45 ± 4.63	606.64 ± 4.56	591.05 ± 4.48	595.40 ± 4.60	672.75 ± 4.82	644.67 ± 4.71	558.85 ± 4.82	545.87 ± 4.66	574.03 ± 4.76	564.37 ± 4.61	664.54 ± 4.99	630.22 ± 4.72
Pb	33.30 ± 5.18	21.35 ± 4.78	32.60 ± 3.59	32.94 ± 3.52	35.03 ± 3.45	32.01 ± 3.44	33.27 ± 3.44	31.93 ± 3.41	32.55 ± 3.81	31.13 ± 3.62	36.65 ± 3.86	37.75 ± 3.83	31.77 ± 3.69	31.44 ± 3.47

* soils treated with H_2O_2

TE's µg/kg	Examples													
	2	2*	3	3*	5	5*	7	7*	14	14*	15	15*	19	19*
	-	H_20_2	-	H_20_2	-	H_20_2	-	H_20_2	-	H_20_2	-	H_20_2	-	H_20_2
Mg	4075.26 ± 1241.90	5907.59 ±1148.31	9045.79 ± 947.60	9929.36 ± 935.05	9312.32 ± 936.71	9131.77 ± 931.21	8790.84 ± 926.40	8936.29 ± 931.79	10458.02 ± 1039.71	10504.26 ± 1025.38	8948.58 ± 997.25	10004.46 ± 986.15	8966.23 ± 955.95	8475.28 ± 918.93
Al	50450.23 ± 727.31	47892.36 ± 695.58	62506.51 ± 619.01	65533.68 ± 617.75	61951.42 ± 615.44	62315.55 ± 617.48	61018.01 ± 617.70	63244.43 ± 618.00	59150.57 ± 654.26	59039.76 ± 647.29	64064.69 ± 644.39	66564.68 ± 641.45	63768.31 ± 628.25	59604.42 ± 614.39
Si	283699.51 ± 1010.90	299754.68 ± 1025.51	363497.80 ± 813.13	360118.55 ± 796.90	365383.18 ± 803.35	365073.07 ± 808.81	365874.17 ± 809.92	363927.98 ± 797.10	335105.62 ± 897.70	338989.76 ± 882.98	354781.16 ± 848.45	352992.33 ± 821.18	361166.94 ± 834.13	368855.25 ± 813.10
P	11692.33 ± 517.82	12448.17 ± 502.86	2525.06 ± 360.98	2811.42 ± 358.86	1002.62 ± 355.54	1271.69 ± 361.62	1719.40 ± 366.91	2399.29 ± 359.09	10355.16 ± 427.65	10938.10 ± 432.06	1563.32 ± 377.56	2306.74 ± 364.19	837.62 ± 365.10	479.17 ± 367.09
S	599.15 ± 42.36	456.19 ± 39.51	180.33 ± 28.66	78.37 ± 27.60	139.38 ± 28.03	88.42 ± 27.69	191.44 ± 28.44	104.97 ± 28.36	301.10 ± 31.95	215.65 ± 31.75	280.28 ± 29.89	166.88 ± 29.76	170.68 ± 29.23	131.79 ± 27.69
K	15781.77 ± 1861.52	16036.74 ± 1888.46	23280.09 ± 1740.13	22947.47 ± 1687.87	22620.91 ± 1687.72	22604.06 ± 1652.38	22718.34 ± 1721.32	22097.89 ± 1686.08	25904.05 ± 1681.42	24575.58 ± 1613.58	24932.68 ± 1727.89	23261.87 ± 1677.09	23754.90 ± 1762.86	22216.59 ± 1704.79
Ca	144589.00 ± 1416.11	126612.24 ± 1400.22	7850.54 ± 894.70	6894.49 ± 855.77	8989.37 ± 855.58	8159.76 ± 870.30	8394.44 ± 889.78	7677.62 ± 852.85	35924.28 ± 1030.48	31375.12 ± 999.15	13205.46 ± 937.15	12519.82 ± 889.08	10232.14 ± 915.31	8060.45 ± 872.19
Ti	5642.65 ± 387.05	3722.18 ± 356.78	5165.58 ± 262.60	5627.08 ± 260.39	5341.91 ± 258.40	5559.81 ± 260.36	5875.17 ± 268.32	6225.96 ± 265.94	5373.18 ± 279.13	5428.67 ± 268.88	5895.05 ± 275.71	5504.82 ± 265.99	5622.73 ± 275.73	5760.96 ± 262.41
Cr	127.71 ± 95.20	60.25 ± 93.26	97.34 ± 64.61	112.99 ± 61.13	114.18 ± 62.31	105.15 ± 61.64	76.71 ± 63.12	119.58 ± 61.80	127.72 ± 68.05	117.44 ± 64.38	108.86 ± 66.74	96.03 ± 64.32	74.21 ± 67.21	124.61 ± 62.95
Mn	962.12 ± 70.7	731.93 ± 64.35	867.45 ± 50.26	768.56 ± 46.76	608.15 ± 45.84	626.65 ± 45.57	861.45 ± 48.87	755.91 ± 47.88	859.51 ± 51.61	763.36 ± 50.42	752.02 ± 50.78	763.90 ± 48.95	624.47 ± 48.61	542.67 ± 46.07
Fe	20982.27 ± 172.25	17440.18 ± 153.10	23203.24 ± 138.55	23572.55 ± 135.94	22730.28 ± 132.77	23084.43 ± 136.50	22225.87 ± 133.09	21912.60 ± 131.93	25801.91 ± 154.64	24854.74 ± 149.13	28312.32 ± 157.32	27920.52± 152.49	24729.39 ± 144.61	23224.94 ± 136.58
Ni	26.31 ± 17.79	27.56 ± 16.27	20.52 ± 13.09	30.59 ± 12.33	16.93 ± 12.82	24.85 ± 12.07	25.35 ± 12.76	22.58 ± 12.16	34.33 ± 13.75	28.77 ± 12.74	43.16 ± 13.70	30.03 ± 13.05	24.94 ± 13.54	23.70 ± 12.16
Cu	24.65 ± 11.61	19.11 ± 10.60	17.33 ± 8.19	21.40 ± 7.80	21.59 ± 7.52	19.00 ± 7.57	22.13 ± 7.99	17.19 ± 7.76	29.98 ± 8.82	28.47 ± 8.08	38.13 ± 8.56	32.65 ± 8.31	17.21 ± 8.33	17.51 ± 7.67
Zn	126.34 ± 10.06	101.56 ± 8.98	75.77 ± 6.48	73.06 ± 6.29	52.29 ± 5.82	53.62 ± 5.79	83.37 ± 6.43	81.77 ± 6.40	135.57 ± 7.65	125.48 ± 7.22	82.27 ± 6.87	77.11 ± 6.58	57.20 ± 6.44	54.70 ± 5.97
Sr	95.26 ± 2.97	71.51 ± 2.59	103.86 ± 2.23	104.28 ± 2.17	107.88 ± 2.18	107.50 ± 2.19	109.77 ± 2.22	103.31 ± 2.16	115.09 ± 2.46	107.54 ± 2.35	121.42 ± 2.46	114.89 ± 2.33	111.49 ± 2.34	106.61 ± 2.19
Zr	378.29 ± 4.98	268.78 ± 4.08	97.46 ± 2.17	95.99 ± 2.09	111.23 ± 2.19	110.48 ± 2.24	108.87 ± 2.21	99.55 ± 2.13	149.89 ± 2.68	139.80 ± 2.54	124.18 ± 2.45	122.40 ± 2.37	113.72 ± 2.35	108.91 ± 2.23
Sn	464.90 ± 5.86	148.61 ± 3.93	590.45 ± 4.63	606.64 ± 4.56	591.05 ± 4.48	595.40 ± 4.60	672.75 ± 4.82	644.67 ± 4.71	558.85 ± 4.82	545.87 ± 4.66	574.03 ± 4.76	564.37 ± 4.61	664.54 ± 4.99	630.22 ± 4.72
Pb	33.30 ± 5.18	21.35 ± 4.78	32.60 ± 3.59	32.94 ± 3.52	35.03 ± 3.45	32.01 ± 3.44	33.27 ± 3.44	31.93 ± 3.41	32.55 ± 3.81	31.13 ± 3.62	36.65 ± 3.86	37.75 ± 3.83	31.77 ± 3.69	31.44 ± 3.47

* soils treated with H_2O_2

Table 3.Change of color and spectral characteristics of soils under the action of hydrogen peroxide on the example of samples NoNo 14, 15, 16

Sample No according to Table 1	Amount of H_2O_2											
	0 ml			**5 ml**			**10 ml**			**20 ml**		
14	**SOC,%**											
	2.32			2.26			2.10			1.43		
	Munsell HVC											
	7.5YR 3/1			10YR 4/1			10YR 4/2			10YR 5/2		
	CIEL* a* b*											
	L*	a*	b*	L*	a*	b*	L*	a*	b*	L*	a*	b*
	39.78	4.70	9.34	45.26	4.87	9.43	46.55	4.84	10.76	49.76	5.34	11.90
	Integral reflection coefficient ρ_ε (Reflection)											
	111.27			134.34			151.01			180.68		
15	**SOC.%**											
	2.1			2.1			1.74			1.17		
	Munsell HVC											
	2.5Y 3/2			**2.5Y 4/2**			**2.5Y 4/2**			**2.5Y 5/3**		
	CIEL* a* b*											
	L*	a*	b*	L*	a*	b*	L*	a*	b*	L*	a*	b*
	40.3	5.33	10.54	41.25	4.54	10.75	45.59	5.41	12.34	55.97	5.96	15.74
	Integral reflection coefficient ρ_ε (Reflection)											
	120.46			122.82			155.68			215.64		
16	**SOC.%**											
	1.28			0.68			0.56			0.50		
	Munsell HVC											
	2.5Y 4/2			**2.5Y 5/3**			**2.5Y 5/3**			**2.5Y 6/3**		
	CIEL* a* b*											
	L*	a*	b*	L*	a*	b*	L*	a*	b*	L*	a*	b*
	44.32	5	12.23	47.4	4.5	15.45	46.49	6.03	13.45	52.57	6.29	16.98
	Integral reflection coefficient ρ_ε (Reflection)											
	170.16			174.06			185.10			194.48		

Table 4. Parameters of soil organic carbon forecasting models for dry soil samples, treated and untreated with H_2O_2 based on L * a * b * predictors obtained by NixPro

Model	**Parameter**	**Coefficients**	**p-value of parameter**	**p-value of equation**	**RSE**	**R^2**
a) soil samples pre-treated with H_2O_2						
Multiple linear regression with several predictors	Intercept L* a* b*	5.61 -0.08 - 0.06	<0.001 <0.001 >0.05 0.03	<0.001	0.28	0.78
b) soil samples without H_2O_2						
Multiple linear regression with several predictors	Intercept L* a* b*	4.02 -0.03 - -0.06	<0.001 0.01 >0.05 0.01	<0.001	0.27	0.61

Table 5. Parameters of soil organic carbon forecasting models for dry soil samples, treated and untreated with H_2O_2 based on predictors obtained by OurSci Reflectometer

Model	Parameter	Coefficients	p-value of parameter	p-value of equation	RSE	R^2
Soil samples pre-treated with H_2O_2						
Linear regression with one predictor (OurSci)	Intercept Reflection	3.409748 -0.011073	<0.001	<0.001	0.28	0.79
Regression on the main components (OurSci)	PC1	2.756e-01	<0.001	<0.001	0.45	0.80
Soil samples without H_2O_2						
Linear regression with one predictor (OurSci)	Intercept Reflection	3.715649 -0.012183	<0.001	<0.001	0.21	0.68
Regression on the main components (OurSci)	PC1	-2.668e-01	<0.001	<0.001	0.60	0.72

Table 6. Parameters of soil organic carbon forecasting models for dry soil samples, treated and untreated with H_2O_2 based on a set of predictors obtained by OurSci Reflectometer and NixPro

Model	Parameter	Coefficients	p-value of parameter	p-value of equation	RSE	R^2
Soil samples pre-treated with H_2O_2						
Multiple linear regression with several predictors	Intercept Reflection L* a* b*	4.65 -0.007 -0.04 - 0.07	<0.001 0.01 0.05 >0.05 0.01	<0.001	0.27	0.81
Regression on the main components (NIX+OurSci)	PC1	-2.564e-01	<0.001	<0.001	0.46	0.79
Soil samples without H_2O_2						
Multiple linear regression with several predictors	Intercept 365nm 385nm 530nm 587nm 632nm L*	3.30416 2.25664 -1.43845 0.25830 -0.96263 0.66959 -0.03012	<0.001 <0.001 <0.001 >0.001 <0.001 >0.01 0.05	<0.001	0.17	0.87
Multiple linear regression with several predictors	Intercept Reflection L* a* b*	4.21 -0.01 - - -	<0.001 <0.001 >0.05 >0.05 >0.05	<0.001	0.25	0.70
Regression on the main components (NIX+OurSci)	PC1	-2.690e-01	<0.001	<0.001	0.51	0.75

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