JOURNAL OF CHEMICAL EDUCATION

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Article

Digital Tool for the Analysis of UV−Vis Spectra of Olive Oils and Educational Activities with High School and Undergraduate Students

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Cite This: J. Chem. Educ. 2022, 99, 787−798

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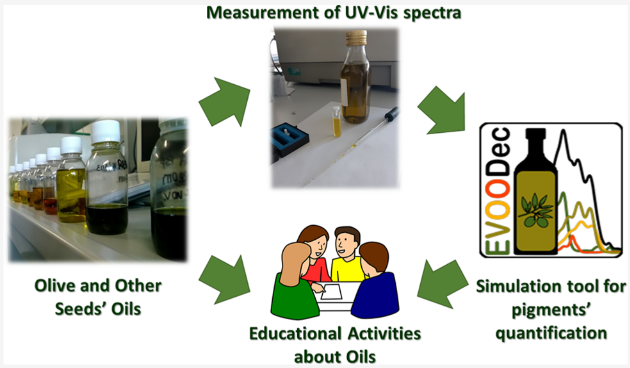


ABSTRACT: UV−vis absorption spectroscopy is one of the most accessible spectroscopic techniques at the high school educational level, and it is usually introduced in analytical chemistry courses due to its high versatility and to the wide range of applications in many fields of chemistry. Within this framework, we have developed an easy-to-use "simulation tool" to identify and quantify the main pigments in a relatively complex food matrix, such as olive oil and seeds' oils. This digital software, freely available, can be used by high school students and first-year undergraduate students to analyze the UV−vis absorption spectrum of olive oils recorded in the bulk without any chemical treatment. In this paper, we are reporting the basic principles of the spectroscopic method and the way to use the "simulation tool" with several examples and explanations that are useful for students and teachers. In the second part of the paper, several examples of activities about the chemistry of olive oil, realized with the fifth classes' students of a high school technical institute (K−12 level) and undergraduate students of an introductory course in spectroscopy in the second year of the Chemistry Degree Course, are reported. These activities were performed partially face-to-face and partially in distance learning mode during the COVID-19 pandemic. The main learning outcomes, methodological issues, and students' feedback resulting from these experiences are reported and commented on, showing the potential of the simulation tool for educational purposes.

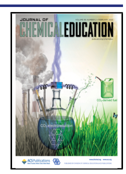
KEYWORDS: *High School/Introductory Chemistry, Analytical Chemistry, Interdisciplinary/Multidisciplinary, Computer-Based Learning, Distance Learning/Self Instruction, Applications of Chemistry, Spectroscopy*

■ INTRODUCTION

Spectroscopy at High School and First-Year Undergraduate Educational Levels

In the scientific literature about chemical education at high school and at first-year undergraduate educational levels, several papers and reviews[1−15] have been published reporting spectroscopic experiments with hands-on spectroscopes, colorimeters, and other spectroscopic instruments to enhance student learning of basic concepts of physical chemistry and analytical chemistry. Most of these educational-designed research activities deal with UV−vis absorption and/or emission spectroscopy, except for a few reported detailed experiences on how to introduce the following to beginners: infrared (IR),[9,13] nuclear magnetic resonance (NMR),[8,9] and Raman[14] spectroscopic techniques. UV−vis spectroscopy is the most accessible to high school students with respect to other spectroscopies for several reasons: (i) they already experience visible light in everyday life;[16] (ii) basic principles of light and optical phenomena, such as reflection and refraction ones, can be explained without referring to complex scientific concepts and mathematical tools;[17] (iii) there are lots of applications of UV−vis spectroscopy that are included in the chemistry curriculum and analytical chemistry courses.[4,5] However, there is still evidence of difficulties and misconceptions encountered by students when dealing with UV−vis spectroscopy due to abstract and theoretical explanations used by teachers, on one side, and to the lack of practical/laboratory activities, on the other side.[4,5,16] This last aspect is also related to the fact that traditional spectroscopic instruments may be absent in high schools or their use is limited or denied to students due to their cost. A way to overcome this limitation, as reported in several papers[1−3,6,7] and in a very complete and interesting recent review,[4] is to let students build their own instruments for direct

Received: September 27, 2021
Revised: December 29, 2021
Published: January 13, 2022



observation of the emission spectrum of different light sources in the visible or UV−vis spectral ranges. Spectrophotometers and colorimeters, either those commercially available or homemade ones, can be used to observe and register the absorption spectrum of colored solutions, as well as to derive the Lambert−Beer law and for quantitative measurements of the concentration of pigments and chromophores in solution.[10−12] These laboratory activities are fundamental in basic courses of analytical/general and physical chemistry for undergraduate students, too. In the literature, there are many examples of different applications of UV−vis spectroscopy in analytical chemistry lab,[18] inorganic[19] and organic[20,21] chemistry laboratories, as well as, more recently, in industrial and green chemistry lab.[22,23] One of the advantages of using UV−vis spectroscopy for educational purposes is the possibility to face up real-life problems or aspects of chemistry strictly related to society. As an example, recent works reporting UV−vis spectroscopy laboratory activities applied to metal determination in water[24] and the quantification of glyphosate, one of the most widely used herbicide on earth,[25] can be cited as representative of this aspect. As remarkably reported by Talanquer[26] in describing the 10 levels of learning within the tetrahedral model of chemical education,[27] inquiry-based and problem-solving educational activities based on UV−vis spectroscopy can be used to help students in reasoning about chemical implications and putting chemistry in a real context.

Digital Tools and Technological Aids During the COVID-19 Pandemic

During these past years 2020 and 2021, due to the closure of schools and universities in many countries around the world due to the COVID-19 pandemic,[28] teachers had to make intensive use of digital tools, such as internet and e-learning platforms, and this big change toward distance teaching and learning modalities involved chemistry, too. As a result, hundreds of papers reporting homemade laboratory activities, distance educational experiences exploiting digital resources and tools, and chemical education reflections at different school levels have been produced. Some of them were also collected by this *Journal*, in the special issue *Insights Gained While Teaching Chemistry in the Time of COVID-19*.[29] The use of augmented and immersive reality[30] and virtual laboratories[31−33] offered additional teaching instruments used to introduce different chemical concepts and themes at high school and undergraduate educational levels. Moreover, during the long period of closure of schools and universities, and, in general, in distance education modalities, the possibility to use digital tools and platforms for educational activities is an important aspect to enhance student participation and engagement. To this aim, the development of specific and user-friendly "digital tools" to help students' analysis and interpretation of data is an important issue.

In the present work, an easy-to-use simulation tool was developed to analyze UV−vis spectra of different vegetable oils, and specifically extra-virgin olive oils (EVOOs), recorded in the bulk, without any chemical or physical treatments, in terms of the main natural pigments. The mathematical and chemical−physical bases of the UV−vis spectroscopic deconvolution method were published in previous works,[34−36] and several scientific research studies[37−39] have been carried out demonstrating the utility of this method in order to discriminate extra-virgin olive oils produced in different geographical areas, produced in different harvest years, and produced from different olive cultivars. These previous scientific papers[34−39] report the results of about 10 years of research in the field of pigments in virgin and extra-virgin olive oils. On the analytical point of view, this spectroscopic method has been validated,[34,37] and its ability to quantify main pigments in extra-virgin olive oils has been compared with standard techniques, such as high-performance liquid chromatography (HPLC),[37] showing its robustness and reliability for fast analysis of olive oils. From the educational point of view, the theme of olive oils and in general vegetable oils has several advantages, since it allows teachers to explore different aspects of chemistry, such as food chemistry, natural compounds, and the healthy and nutraceutical properties of olive oils.[40−45] Olive oil chemistry is indeed an interesting topic due to several educational implications. It can be used to discuss and compare different analytical methods for the chemical characterization of a complex matrix,[43] to describe the saponification reaction, and to show some applications about sustainability in chemistry, such as the conversion of vegetable and plant oils into biodiesels.[44,45]

In this work, we describe the basis of the "simulation tool", some examples of how to use it with high school and first-year undergraduate students, and a scheme of educational activities about olive oil chemistry planned and realized during the COVID-19 pandemic.

■ DESCRIPTION OF THE SIMULATION TOOL AND HOW TO USE IT

The analysis of UV−vis spectra of a complex matrix containing more than one component requires a spectral deconvolution. The mathematics behind the spectral deconvolution is based on a matrix formalism.[34,46] Usually, this formalism is not suitable for high school students that are not familiar with matrix tools and operators. However, principles of the spectral deconvolution can be illustrated starting from the students' background knowledge about spectroscopic concepts. To introduce students to the topic, it is useful to recall the Lambert and Beer's law[47] and its application to a mixture of two or more absorbing species in solution. As demonstrated in previous works,[34−39] if we suppose that the UV−vis absorbance spectrum of olive oil is due to the presence of N pigments, the total absorbance at a given wavelength, $A(\lambda)$, can be written as a sum of contributions:

$$A(\lambda) = \sum_{i=1}^{N} A_i(\lambda) = \varepsilon_i(\lambda) b C_i \tag{1}$$

in which $\varepsilon_i(\lambda)$ is the absorption coefficient of the ith pigment at the wavelength λ, b is the optical path, and C_i is the concentration of the ith pigment in solution. In our case, the absorption spectrum of olive oil is available from experiments, but the concentration of the single pigments is unknown. The goal of the deconvolution procedure is to look for the correct combination of pigments' concentration C_i resulting in a total calculated spectrum, $A_{\text{calc}}(\lambda)$, as close as possible to the experimental one, $A_{\text{exp}}(\lambda)$. The quality of the mathematical deconvolution procedure can be evaluated by computing the R^2 parameter, here defined as

$$R^2 = 1 - \frac{\sum_\lambda (A_{\text{exp}}(\lambda) - A_{calc}(\lambda))^2}{\sum_\lambda (A_{\text{exp}}(\lambda) - \overline{A_{\text{exp}}(\lambda)})^2} \tag{2}$$

where $\overline{A_{\text{exp}}(\lambda)}$ is the average value of the experimental absorbance over the whole spectral window. The method is similar to a fitting procedure that students commonly use for the regression analysis of experimental data. It is worth notice that

https://doi.org/10.1021/acs.jchemed.1c01015
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the agreement between $A_{calc}(\lambda)$ and $A_{exp}(\lambda)$ should be the best for all the wavelengths included in the considered spectral window; in fact, a change in one of the pigments' concentrations in principle may affect $A_{calc}(\lambda)$ at all wavelengths, leading to a multivariate regression model. In order to let students easily access to the spectral deconvolution, we developed an easy-to-use digital tool called *EVOODec*, which is designed for both expert and novice users and can be used for pigments' quantification with high analytical standards[34−39] in extra-virgin olive oils (EVOOs). As recently demonstrated,[37] the deconvolution method can be used to study pigments' content and evolution during storage, from "freshly pressed" to "on-the-shelf" EVOOs. The software logo is shown in Figure 1.

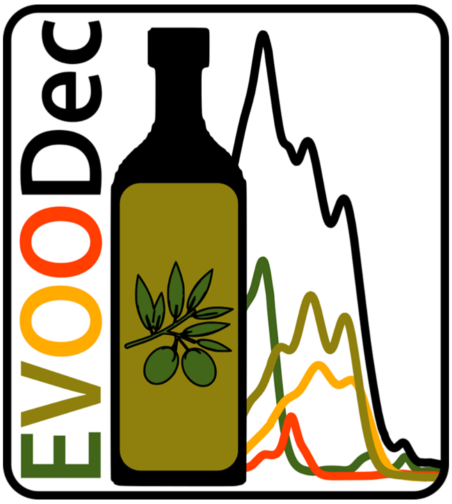

Figure 1. Logo of the software used to analyze the near UV−vis spectrum of olive oil in terms of main pigments.

EVOODec is a Python3 program with a user-friendly graphical user interface (GUI) developed by using the Tkinter library.[48] The software is freely available at the link https://github.com/sandroj87/EVOODec/releases.

In the following, we report how to use the digital tool to analyze the UV−vis spectra of olive oils and, as will be shown in the next sections, other vegetable oils. First, the experimental UV−vis spectrum of the EVOO sample should be recorded (see the experimental protocol reported in the Supporting Information); then, the corresponding file of the experimental spectrum has to be imported in *EVOODec*, and the deconvolution procedure begins. The user can select the appropriate spectral window and choose the pigments for the deconvolution (several natural pigments can be chosen as described in the following sections). The software will automatically produce and display the best calculated spectrum obtained by summing the absorbance of the selected pigments "weighted" for the concentration values resulting from the deconvolution procedure. The workflow is summarized in Figure 2.

The design of the program interface drives the user step-by-step in the deconvolution procedure with clear selectable options and real-time graphical feedback in response to any parameters' change. The main window is organized into two areas: the input area (left side) that contains all selectable options to set up the deconvolution, and the output area (right side) where the results are shown. The output area is divided into a plot region, where the experimental spectrum and that

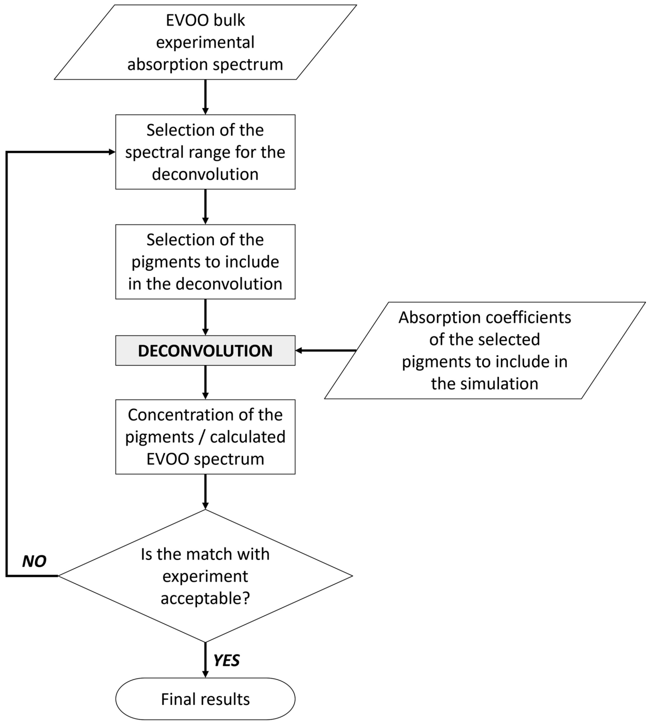

Figure 2. Workflow for the EVOO spectral deconvolution.

obtained from the deconvolution are shown, as well as two separated text boxes reporting the pigments' concentration results and other program notifications. The main window of *EVOODec* is shown in Figure 3.

The installation and first-use guides of the *EVOODec* simulation tool are available in the Supporting Information. Here, we explain how the program works. Once the program is opened, a default experimental EVOO spectrum is loaded and the plot area appears: this is useful to perform some preliminary tests. Anyway, any other spectrum can be easily loaded at any time by the user.

To obtain the spectral deconvolution, the user can follow the step-by-step configuration as suggested by the blue boxes from the top to the bottom of the input area (see Figure 3):

- **Step 1. Selection of Input Data Files.** By default, the reference data file containing the single pigments' absorption coefficients is loaded. The list of the pigments available for the deconvolution is automatically shown in the pigment control panel. In particular, the following pigment's molar extinction coefficients have been implemented in the last version of the software: β-carotene (b-CAR), lutein (LUT), neoxanthin (NEX), chlorophyll a (Chl-a), pheophytin a (Pheo-a), chlorophyll b (Chl-b), and pheophytin b (Pheo-b).[34−36] Note that the first substance of the list, i.e. triolein (TRIO), is not a pigment, but it is representative of the EVOO matrix, namely, the fatty acids and triglycerides (98−99% of EVOO constituents), and it is necessary to simulate the spectral baseline.[34−36] The inclusion of triolein is indeed strongly recommended in the simulation to obtain reliable results. Each pigment will be displayed in the plot with a different and customizable color. The experimental data set can be loaded by clicking on *Load EVOO spectrum*. After data loading, the experimental spectrum appears in the plot area, and it is represented by gray dots

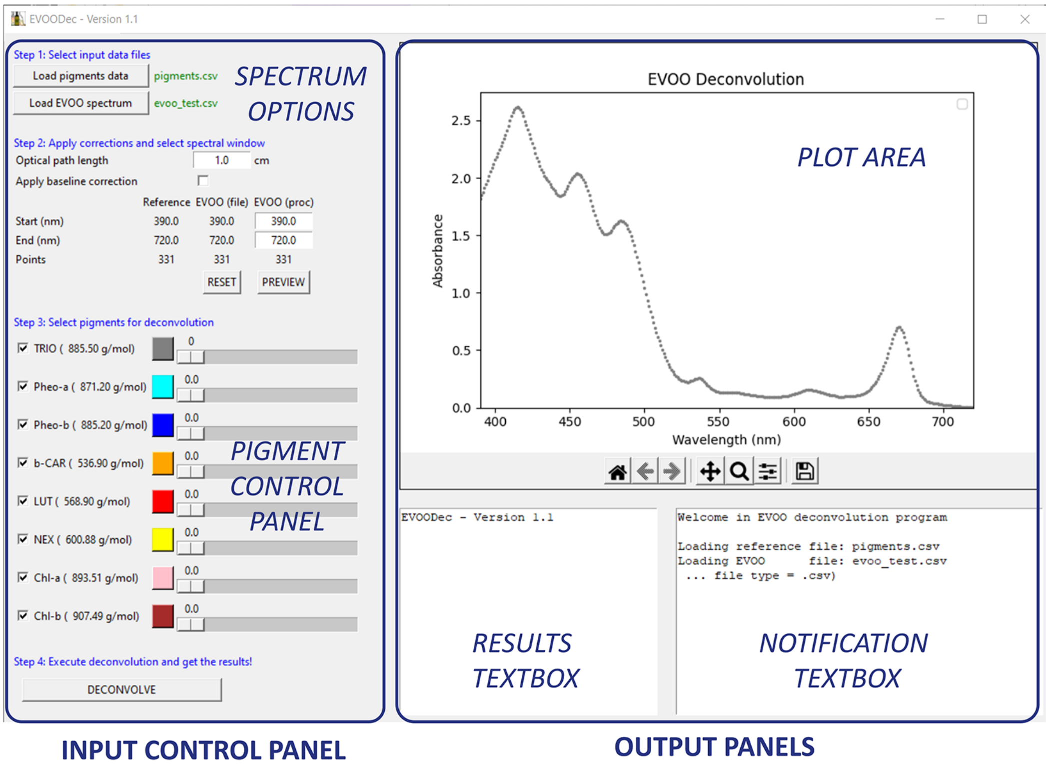

Figure 3. EVOODec graphic user interface. The main working areas are highlighted.

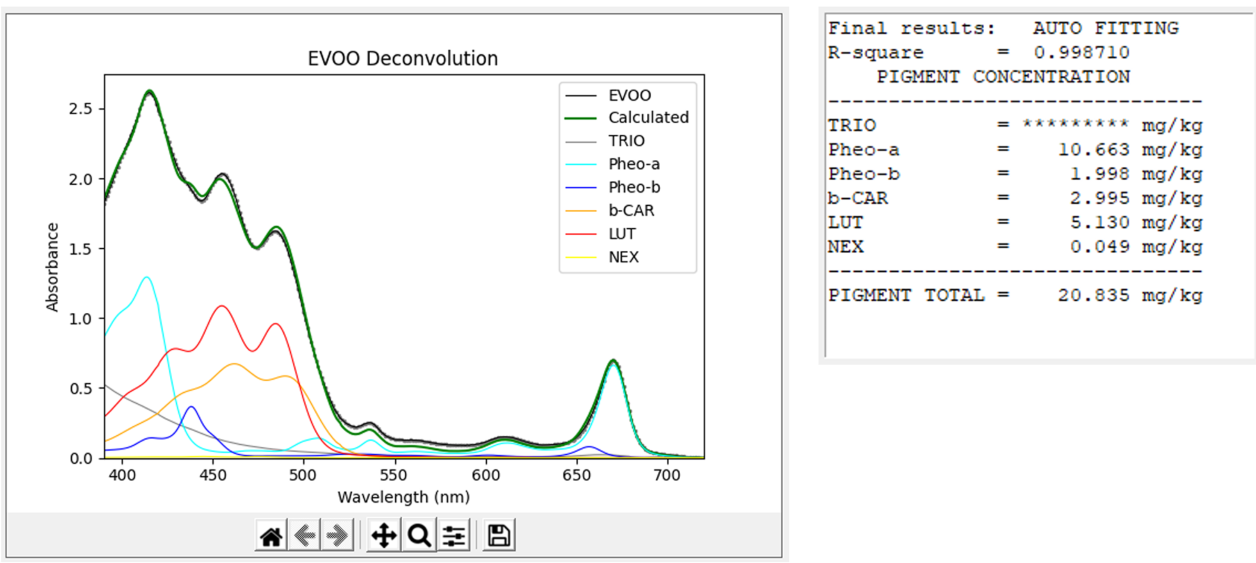

Figure 4. Results of the deconvolution obtained for the EVOO reference data set. The black line corresponds to the experimental spectrum of a reference olive oil sample, and the green line refers to the calculated spectra from the deconvolution. Other colored lines correspond to the contributions of the selected pigments (pheophytin a, pheophytin b, β-carotene, lutein, and neoxanthin); the gray line is the contribution of triolein.

corresponding to absorbance/wavelengths experimental points.

- **Step 2. Selection of Spectral Window.** The program automatically selects the active spectral range for the deconvolution as the maximum overlap between the wavelength ranges of the reference pigment's absorption data and the experimental spectrum of EVOO. If needed, the user can choose a different subset of wavelengths. If the two data sets are not recorded with the same resolution, the program uses a *spline* interpolation to obtain data sets with the same resolution. In fact, as reported in the Supporting Information, the optimal spectral resolution of the olive oil spectrum is at least 1.0 nm; however, if the instrument has a lower resolution, the program automatically interpolates the experimental data in order to get a spectral resolution of 1.0 nm. A baseline correction can also be added to shift the minimum value of absorbance of the experimental spectrum to zero. This

https://doi.org/10.1021/acs.jchemed.1c01015
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is particularly convenient if the EVOO is not completely transparent. As reported in the Supporting Information, a way to solve this problem is to filter the olive oil sample before the acquisition of the UV−vis spectrum.

- **Step 3. Selection of Pigments.** At this step, the user performs the selection of pigments to be considered in the deconvolution by flagging the corresponding checkbox. A reasonable starting point for a commercial EVOO (also denoted as "on-the-shelf" EVOO) is to include the effect of the matrix simulated by triolein (TRIO) and four main pigments: pheophytin a (Pheo-a), pheophytin b (Pheo-b), β-carotene (b-CAR), and lutein (LUT). As demonstrated in previous studies, in fact, the concentration of chlorophylls is relatively low, and they can be neglected in a first approximation.[34−39] The case of "freshly pressed" olive oils is different,[36] as will be shown in the next sections of the paper. The sliders next to the pigment names can be used for a manual simulation procedure: moving the slider from left to right as the concentration of the pigment increases as well as its contribution to the total absorbance in the calculated spectrum displayed on the right side.
- **Step 4. Execute the Deconvolution.** Finally, the user can run the deconvolution by pressing the *DECONVOLVE* button. The results are shown in the plot using the following color-scheme code: (a) The green thick line corresponds to the total calculated absorption spectrum; (b) the colored thin lines correspond to the contribution of each selected pigment to the total spectrum. The pigments' concentrations, expressed as mg/kg, for olive oil are reported in the result panel below the plot and can be easily copied and pasted to an external worksheet.

The result of the deconvolution procedure applied to the preloaded EVOO spectrum by including the pigments suggested as a starting point in step 3 is shown in Figure 4. In this case, to obtain a better agreement between the calculated and experimental spectrum, we also added a fifth pigment, namely, neoxanthin (NEX),[35] to the fitting.

Users may also experience the effect in changing the concentration of one or more pigments on the total calculated spectrum using the manual deconvolution mode by acting on the concentration sliders. The manual deconvolution mode can be effectively used by the teacher to introduce the physical meaning of the deconvolution before exploiting the automatic mode (see suggestions reported in the didactic sequence reported in the next section). In this way, students may experience the complexity of a multivariate regression problem, get a feeling with the simulation, and check the sensitivity of the method in response to changes of the input parameters, avoiding math anxiety.[49]

■ PROJECTS ON EXTRA-VIRGIN OLIVE OIL WITH HIGH SCHOOL AND UNDERGRADUATE STUDENTS

In this section of the paper, we introduce two projects on EVOOs performed: (i) with two classes of high school students (K−12 level) and (ii) with undergraduate students attending an introductory course about spectroscopy ("Physical Chemistry and Laboratory").

Project about Olive Oil Chemistry for High School Students of the K−12 Level

The analysis of the content of pigments in EVOOs is part of a wider project about the chemical characterization of olive oil samples. This project has been proposed to the students attending the fifth year (corresponding to the K−12 level) of the high school "*Carlo Cattaneo*", a technical institute placed in San Miniato (Pisa, Italy). The school is indeed located in a part of Tuscany (a central region of Italy) where there is a long tradition for the cultivation of olive trees and the production of high-quality extra-virgin olive oils. The project has been carried out in October, November, and December of 2021, during the second wave of the Italian COVID-19 pandemic. For this reason, only the practical laboratory activities have been performed in the presence of all students at school, whereas all other activities and lessons have been carried out with distance learning modalities.

The project flowchart shown in Figure 5 starts with laboratory experiments, in which classical methods (such as determination

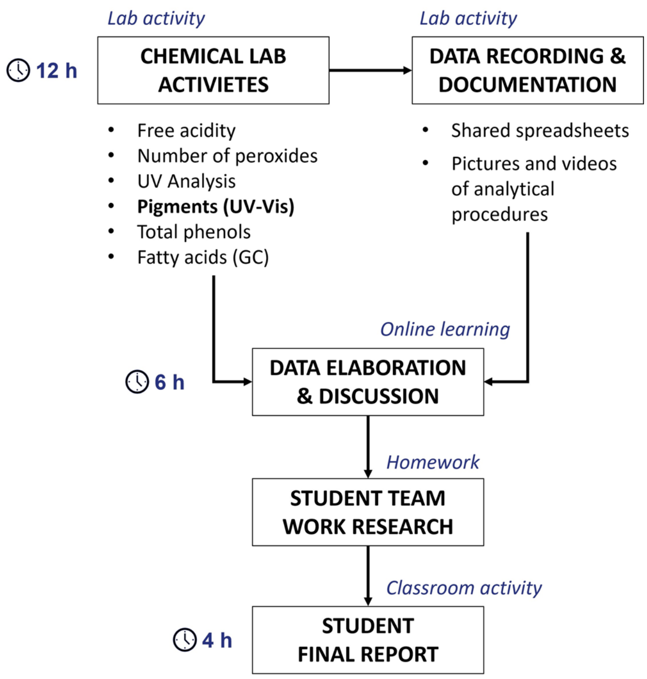

Figure 5. Flowchart of EVOO project carried out with high school students (K−12 level).

of free acidity and number of peroxides) and instrumental analytical techniques (UV−vis spectroscopic analysis to determine K232 and K270 index and gas-chromatographic analysis) were applied to different commercial and fresh EVOO samples.[50] Olive oil is a very good food matrix to improve students' analytical skills because it gives the possibility to apply standard analytical techniques,[41−43] practiced in the previous school years, to a real sample with a relatively high level of complexity. This opens the possibility to explore several basic chemical concepts, such as the physical chemistry of water/oil systems, principles of separation techniques, such as the extraction of single classes of chemical compounds from complex matrix, and how to treat a real sample before performing a chemical analysis and so on.

The experimental data acquired in the lab are usually stored in a class-shared spreadsheet, and the key steps of the experimental procedures are documented by pictures or short videos shared in a cloud with the class. The laboratory activities are mainly focused on developing the practical skills of the students, as required by the chemical curriculum of the technical institute. Due to the limited time, methods and data discussion were

https://doi.org/10.1021/acs.jchemed.1c01015
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postponed in a second online learning step. For this reason, the documentation work performed in the chemical laboratory represents a valid support for the student to "relive" the experience during the discussion.

After the online data analysis and theoretical background discussions performed at a distance during video lessons, we proposed a teamwork research activity regarding several subtopics concerning EVOOs. In particular, the three main topics assigned to each group were (a) the olive oil world (production, legislation, falsification, fraud, etc.), (b) the olive oil chemical analysis (discussion and data elaboration of one of the analytical techniques proposed in the lab), and (c) the organic chemistry about olive oil and, in particular, triglycerides.

The conclusion of the project of each group of students consists of the preparation of a report (edited by the members of the group in a collaborative way by using a shared document) and, finally, a brief oral presentation to share the research report with other students.

Despite the particular situation due to the COVID-19 pandemic, this project included a large section devoted to laboratory experimental activities conducted mainly in person, supported by prelaboratory activities, and data analysis and discussion were performed during synchronous and asynchronous online activities. The series of steps reported in the flowchart of Figure 5 takes into account the role of laboratory learning environments, which has to be considered a complex learning environment,[51] where chemical and other scientific knowledge, different skills, and students' attitudes are integrated.[52]

The students' feedback and the effectiveness of the activity related to the analysis of the UV−vis spectra of olive oils by using the *EVOODec* tool are discussed in the final part of this paper.

Laboratory Activity about UV−Vis Spectroscopy for Undergraduate Students

During the last semester (from February to May 2021), about 35 students attending the course of "Physical Chemistry and Laboratory" at the second year of the "Laurea" Degree in "Industrial and Environmental Chemistry" (analogous to the Eurobachelor in Chemistry) at the University of Pisa in Italy[52] have used the *EVOODec* simulation tool to analyze the UV−vis absorption spectra of several olive and other vegetable oils. This Degree Course has more applicative purposes with respect to the Degree in Chemistry. During the Physical Chemistry and Laboratory course, students should learn the basic principles of spectroscopy, and learn and practice the main applications of several spectroscopies, such as UV−vis absorption spectroscopy, fluorescence, and infrared spectroscopy. The first part of the course (about 24 h) deals with the introduction of principles of quantum mechanics and the chemical−physical theory of spectroscopy. The second part of the course (24 h of theory and 45 h of laboratory) is about instrumentations and data analysis, examples of applications of spectroscopy to different areas of chemistry, resolution of numerical exercises, and discussion/elaboration of the laboratory activities. Due to the second lockdown in Italy during the second semester of the academic year 2020−2021, all courses were in distance modality except for the practical laboratory activities, performed in person. With respect to usual laboratory activities, this year students could access to the laboratory in small numbers, and single experiences were repeated for each student (no cooperative or group activities were allowed in person). The laboratory activity concerning UV−vis spectroscopy was centered on the analysis of vegetable and olive oils. Each student could register his/her own spectra choosing among a series of available vegetable oils. This part of the activity was in person, and each student had about 1 h to perform measurements by using a standard UV−vis spectrophotometer. Before going to the lab, the basic principles of UV−vis spectroscopy and relative instrumentations were introduced to students during remote lessons, as well as the basics of safety and correct behaviors in the lab. After the laboratory activity, the spectra recorded by the students were shared in a common folder, and all other educational activities ware performed in the remote learning mode, through "Microsoft Teams" and the e-learning Moodle platforms provided by the University of Pisa. During the lessons which followed the laboratory activities, the teacher showed the mathematical principles of the deconvolution model to analyze UV−vis spectra; showed a video tutorial describing how to download, install, and use the *EVOODec* tool; and gave basic information about the chemistry of natural pigments present in vegetable and olive oils. Compared to high school students, in the case of undergraduate students, during all steps of the data analysis, from the recording of the UV−vis spectra to the conversion to the correct file format and spectral analysis by using the *EVOODec* tool, students should have to work without the teacher's help, and they had to solve eventual problems by themselves. A final step of the activity for undergraduate students included cooperative work, in remote mode, where groups of 3−4 students had to discuss together the obtained results and prepare a scientific report about the analysis of pigments in olive oils and other vegetable oils by means of UV−vis spectroscopy.

As discussed in the following, several examples of activities on olive oils and other vegetable oils can be proposed to students, in which the *EVOODec* simulation tool represents a helpful educational tool.

■ EXAMPLES OF ACTIVITIES WITH THE "EVOODEC" SIMULATION TOOL

In this section, we describe two examples of activities on olive oils that can be performed by using the *EVOODec* simulation tool. Relative original files to be used as examples by the teachers can be found in the "spectra" folder included in the software package.

First Example of Application of the Simulation Tool: Fresh versus On-Shelf Extra-Virgin Olive Oils

Among the interesting applications of the present spectroscopic method having educational implications, we propose the analysis of extra-virgin olive oils having different "age". It is well-known, in fact, that the chemical composition of oils changes during the storage, and it depends on external conditions, such as light, oxygen, or heat exposure.[36,50] Moreover, even if the storage conditions are optimal, namely, the olive oil sample is left in the dark, and stocked in sealed bottles, at temperatures lower than 5 °C, olive oil pigments' content evolves during time.[50,53] This aspect should be rather clear to students who observe the color changes from fresh olive oils after a few days from the production (i.e., the color is green-yellow), to olive oil samples 2−3 months after the production (i.e., the color is brown-yellow). The color change reflects the spectral change, which is mainly due to the pheophytinization process:[36,50,54,55] the conversion of chlorophylls into pheophytins. This process can be indeed followed by measuring (and analyzing) the UV−vis absorption spectra of olive oils at different times. As observed in Figure 6, the major differences among olive oils with different "ages" are observed in the spectral region from 400 and 500 nm, where the more intense absorption bands of chlorophyll a and chlorophyll b, as well as pheophytin a and pheophytin b, show the larger shifts. The EVOO sample shown in Figure 6, for instance, is a relatively fresh olive oil, and this can be noticed by the fact that the deconvolution of the UV−vis spectrum by using only carotenoids and pheophytins is not satisfactory (red curve in Figure 6b).

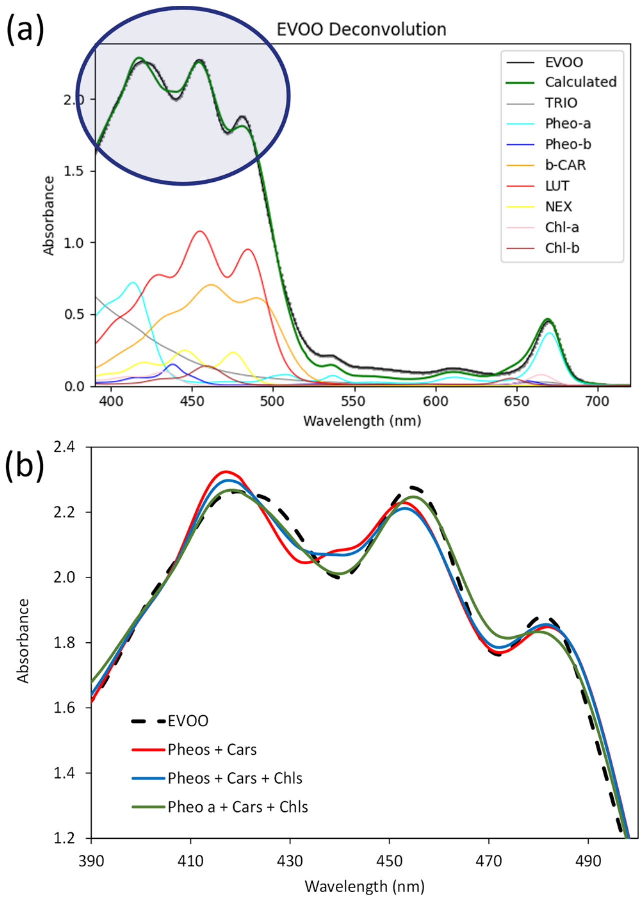


Figure 6. (a) Example of UV−vis spectrum of an EVOO sample after a few days from its production. Green solid curve represents the best deconvolution of the experimental spectrum (black curve), and the reference pigment components are also reported in different colors. (b) Superposition among the experimental spectrum of the EVOO sample (black dashed curve) and the calculated spectra (solid curves) obtained with different combinations of reference pigments, as indicated in the legend, in the spectral region from 390 to 500 nm. Pheos, Cars, and Chls indicate the sums of pheophytins, carotenoids, and chlorophylls, respectively.

The best spectral reproduction is obtained only if chlorophyll a and chlorophyll b are included among the pigments' reference spectra. In particular, the best spectral deconvolution is obtained by using chlorophyll a, chlorophyll b, pheophytin a, β-carotene, lutein, and neoxanthin (green curve in Figure 6b). If the readers are interested in a detailed study of UV−vis spectral evolution over time, ref 36, which contains a kinetic study too, is suggested either for research or for educational purposes. During the activity proposed for high school and undergraduate students, the pigments' content obtained by analyzing the UV−vis absorption spectrum in different olive oils can be compared and discussed. Moreover, students can estimate the olive oil's "age" by taking into account the concentration of chlorophylls, if present. It is also possible to study the evolution of pigments over time by analyzing the spectral data obtained for EVOO samples in a period of time of several months or stored under different conditions, such as different temperatures, light conditions, or oxygen exposures. As demonstrated in this recent paper,[36] pigments' degradation follows mainly a first-order kinetics, whose math is accessible to high school students, too.

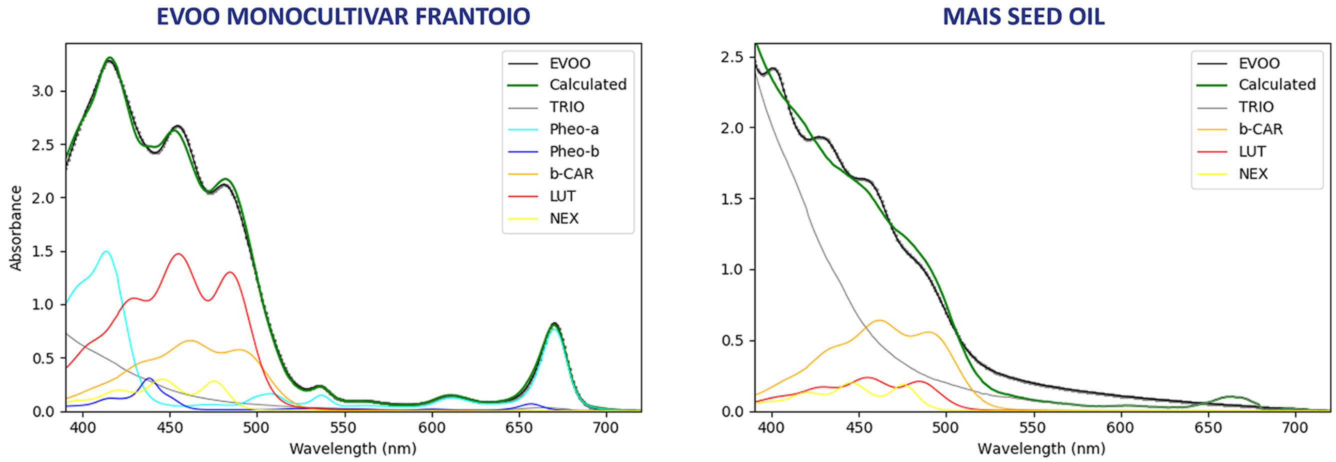
Second Example of Application of the Simulation Tool: Extra-Virgin Olive Oils versus Other Vegetable Oils

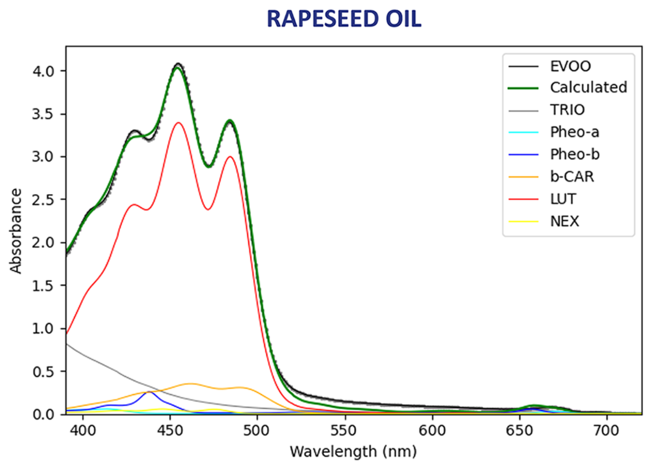
Another school activity related to the topic is the application of this method to other vegetable oils than olive oils. The pigments' content is indeed very different among vegetable oils, such as soybeans and sunflower oils, nuts and corn seed oils, and rapeseed and linseed oils. All of these vegetable oils are edible, or they are used for frying and cooking, so they are an interesting topic in food chemistry. Moreover, among common adulterations of extra-virgin olive oils,[42] the mixing of low-quality olive oils with different percentages of vegetable oils still represents a challenge, as demonstrated by the numbers of scientific publications about the topic.[53−55] As reported in Figure 7, the quantitative analysis of the UV−vis spectra of different oils can give interesting information about the pigments' content.

An almost perfect fit (R^2 of 0.9991) is obtained for the EVOO sample made from monocultivar *Frantoio* olives (a typical cultivar from Tuscany, Italy), where β-carotene, lutein, and neoxanthin are used among carotenoids, and pheophytin a and pheophytin b are used among chlorophylls' derivatives. The mais (corn) seed oil on the contrary results in the worse fitting, and this is due to the small amounts of pigments as denoted by the light-yellow color of the oil: the total content of pigments is about 5 ppm, mainly due to carotenoids. A peculiar vegetable oil is that obtained from rapeseeds, whose spectrum reveals the presence of a large quantity of lutein (about 16 ppm), much larger than that contained in olive oils. On the other hand, rapeseed oils do not contain any chlorophyll derivatives (in the limit of quantification). A further activity connected with this one consists of the preparation of blends of olive oils with vegetable oils and the study of the pigment composition changes with respect to the percentage of oil mixed together.[34−36,55] As discussed so far, the number of activities and education aims of the present tool cover several main topics in chemistry.

■ LEARNING ACTIVITY, EVALUATION, AND DISCUSSION

In general, the analytical techniques experienced by the students at high school and first-year undergraduate educational levels usually require a sample treatment, chemical and/or reagent consumption, and relatively time-consuming procedures. On the contrary, the spectroscopic method reported here to determine pigments' content in olive and other vegetable oils is a nondestructive method, and it does not require any treatment (at least a simple filtration in case of turbid oils), or any solvent usage, allowing for a cost reduction and more sustainability. Also, it is a very fast method. For these reasons, during the pilot study, it was interesting to discuss with the students the differences, advantages, and disadvantages, of the spectroscopic method for the pigments' analysis based on the deconvolution of UV−vis spectra and more standard spectroscopic methods. In the present paper, we have reported a didactic sequence for high school students, in which the





DECONVOLUTION RESULTS

	EVOO MONOC. FRANTOIO	MAIS SEED OIL	RAPESEED OIL
R^2	0.9991	0.9902	0.9988
Pheo-a	12.3	-	0.5
Pheo-b	1.7	-	1.4
b-CAR	2.9	2.8	1.6
LUT	6.9	1.1	16.0
NEX	1.6	1.0	0.3
∑ Pheos	14.0	0.0	1.8
∑ Cars	11.4	5.0	17.8
Total	**25.4**	**5.0**	**19.7**

Figure 7. UV−vis spectra of an EVOO sample obtained from monocultivar *Frantoio*, a high-quality EVOO sample (on the top left); of a commercial mais (corn) seed oil (on the top right); and of a commercial rapeseed oil (on the bottom left). The best fit obtained by applying the spectral analysis is reported with the contributions of the reference pigments used in the deconvolutions. On the bottom right, a table reports the fitting results in terms of R^2, as a single and as the sum of pigments' concentration (ppm).

EVOODec tool is used for students after a standard UV−vis spectroscopic analysis performed on EVOO samples (namely, K232, K270, and the determination of the polyphenols). Before briefly introducing the theory of the spectral deconvolution approach, based on our experience, we suggest presenting the method starting from a practical application to an EVOO sample by applying a simple tutorial teaching method and possibly within a series of laboratory activities. Within this didactic sequence, the teacher can show the analytical procedure, from the sample preparation to the data elaboration, asking the students to recognize similarities and differences between this method and the classical spectrophotometric methods experienced by the students in the previous lessons. The students' observations can be collected by using a comparative scheme, such as the one reported in Table 1. This scheme was indeed used on the present pilot study with high school students.

As noted during the activities proposed in two fifth classes of a technical institute (K−12 level), where students are familiar with quantitative spectrophotometric determinations, students were really surprised about the strengths of *EVOODec* method, because no calibration curve is needed and especially because many different pigments can be determined in "one-shot" analysis. After an initial discussion, students are usually interested in understanding how it is possible to get these results with this apparent "really easy" approach. At this point, the teacher can explain the physical principles that are at the basis of the method by recalling the Lambert and Beer law and the absorbance additivity principle, as detailed in the previous sections. To introduce the deconvolution method, the teacher can ask different students to perform a "manual" deconvolution of the spectrum by using the slide bars in *EVOODec* (see the INPUT CONTROL PANEL in Figure 3). This is a remarkably effective step that helps students to understand the physical meaning of the deconvolution procedure. Moreover, mathematical aspects beyond the method can be detailed in the math course, showing a realistic connection between chemistry and math. After these activities, students who experienced the

Table 1. Scheme Used for the Collection of High School Students' Observations about Differences among Spectroscopic Methods Used for the Analysis of Olive Oil

Steps/Features of the Methods	*EVOODec* Method	Standard UV−Vis Methods
Sample preparation	Only filtration	Pretreatments (depending to the method)
Calibration curve	Apparently, not needed	Needed
Type of measurement	Scan in a wavelength range	Measure at fixed wavelength
Analytes determined	Many at the same time	One

https://doi.org/10.1021/acs.jchemed.1c01015
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present didactic activity understand how *EVOODec* works, reaching very good marks. In particular, the average mark obtained by the students concerning all aspects that are the object of evaluation (conceptual, scientific, and technical skills) related to the analysis of olive oil UV−vis spectra in terms of pigments' content was 7.6 out of 10 with a standard deviation of 1.7, among a total number of 34 students divided in two classes. The evaluation table used to perform students' evaluation is reported in the Supporting Information, and it is divided into three parts: basic principles of the spectroscopic method, deconvolution tools and how to use it, and technical aspects about the spectral analysis and the *EVOODec* tool. As discussed in the following, the third part was the one which most influenced the students' final evaluation.

The possibility to analyze real samples and to solve real problems is a further advantage of the proposed educational tool. Under the teacher's guidance, students can discuss the obtained results in terms of the evolution of the chemical composition of olive oils, the effect of different seeds, and the fruit or plant origin of vegetable oils on the chemical composition and the effect of storage conditions, as suggested in the examples of the application shown in the previous section.

This educational sequence about the chemistry of olive oil was realized with students from a fifth class of a high school technical institute, and it was performed partially with face-to-face activities and partially with a distance learning mode due to the COVID-19 pandemic. When it was possible, after the first tutorial examples and the following discussion about the basic principles of the method, students were brought to the chemical laboratory to record the UV−vis spectra of olive and vegetable oils, and then they were able to analyze the spectra at home by using the *EVOODec* tool. In the case of high school students, it was useful to show a video tutorial regarding how to use the software. The software package was indeed accessible to all students, who could install and execute it on their own PC. We found that almost all students were able to do all the steps by themselves. About 70% of them have been able to perform the deconvolution of the UV−vis absorption spectra of their EVOO samples and to get the best results in terms of the pigments' composition. The most common problem encountered by students was related to the format of the raw data of the spectrum to be analyzed: the program reads a two column file (wavelengths; absorbance), and students that are not familiar with spreadsheet or other tools to manage CSV data may have some problems to load the input file in *EVOODec*. To overcome this problem, in the case of high school students, it is better to give them the data files in the right format. The teacher can indeed prepare the files as CSV and share them with students, for instance, by using the Google Classroom or other e-learning Moodle platforms. Once the students have been provided the correct files, they are usually able to use them with the *EVOODec* tool and perform the deconvolution by themselves.

The use of the *EVOODec* simulation tool in the frame of a laboratory-centered activity about the chemistry of olive oil allowed us to improve several aspects of the educational activity related to the introduction of spectroscopic methods.

This aspect is important for undergraduate students, too, as we have observed in the case of the students who attended the course "Physical Chemistry and Laboratory" and participated in the activities described in the previous sections. In the case of the activity proposed to undergraduate students in the frame of the introductory spectroscopy course, an anonymous final test was provided to students in order to get their feedback, to check the level of agreement, and to better evaluate the efficacy of the activity. The number of students attending the course during the academic year 2020−2021 and participating in the laboratory activity was 33. Among them, 22 students answered the anonymous survey, before the present paper was submitted, and 18 have already passed the final exam of the course. As reported in Figure 8, all students considered the activity about UV−vis spectroscopy on olive oils useful (45.5%) or very useful (54.5%).

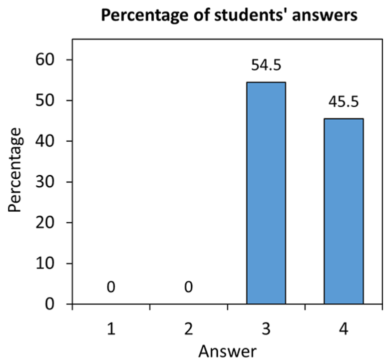

Figure 8. Usefulness of the activity about olive oil for undergraduate students, derived from the analysis of anonymous final test (total number of students, $n = 22$). The plot shows the percentage of students' answers to the following question: "How much of the course devoted to the chemistry of olive oil was of use for your understanding of UV−vis spectroscopy?" Answer 1 indicates "not at all". Answer 2 indicates "not very useful". Answer 3 indicates "useful", and Answer 4 indicates "very useful".

According to students' answers (see Table 2), the usefulness of the activity about spectroscopy of vegetable oils concerns several aspects, such as the quantitative use of UV−vis spectroscopy (i.e., to quantify pigments in olive oils) and the application to real problems and real systems, where several chemical compounds are present giving rise to a complex spectrum. It was interesting to note that students appreciated several parts of the activities about the spectroscopy of olive oils, not only the laboratory in person but also the theoretical explanation performed during remote lessons and the analysis of the spectra through the *EVOODec* tool (see the second question in Table 2). Moreover, a majority of students considered this activity positive or very positive for their preparation and training as future chemists.

As a general remark, during the entire activity about UV−vis spectroscopy of olive oils, we observed a higher interest of students in spectroscopy with respect to the previous years. As can be deduced from students' feedback, this is related to the possibility to solve a "real problem" which is strictly connected to the local context (Tuscany and, in general, the Italian tradition in olive oil production and use) and to the actuality of the problem of fraud in the field of olive oil. As widely reported in the literature, the present work confirms the role of the social and local context in chemistry education and in the efficacy of the activities connected with local culture.[56−58] A general positive perception of chemical laboratory lessons and their utility and a much higher level of multidisciplinary among chemistry, physics, informatics, and mathematics were additional positive aspects of this activity among undergraduate students. Moreover, during both face-to-face and distance activities, students had the chance to work in small groups, for

https://doi.org/10.1021/acs.jchemed.1c01015
J. Chem. Educ. 2022, 99, 787−798

Table 2. Answers of Undergraduate Students Concerning the Activity Performed on Olive Oil and the *EVOODec* Tool During the Course "Physical Chemistry and Laboratory"[a]

Question	Answers (and Percentage of Students Who Answered)				
The activity on the analysis of UV−vis spectra of olive oils was useful for you to...	Better understand the principles of UV−vis spectroscopy (18.2%)	Better understand quantitative applications of UV−vis spectroscopy (45.4%)	Better understand the origin of UV−vis spectra in real matrices (9.1%)	See a real application and usefulness of UV−vis spectroscopy for real problems (18.2%)	Learn how to analyze a UV−vis spectrum and derive quantitative information (9.1%)
Which part of the activity about olive oil was more useful for you?	The preparation of the sample and record of the UV−vis spectrum in the lab (in person activity) (18.2%)	The explanation of the origin of UV−vis spectra of olive oil and the theory at the basis of the deconvolution method (18.2%)	The analysis of the UV−vis spectrum of olive oil by using the EVOODec tool to obtain the pigments' concentrations (9.1%)	For all previous reasons (54.5%)	None of the previous reasons (0%) *No other reasons were added by students*
What is your overall judgment concerning the activity about UV−vis spectroscopy of olive oil?	Very positive for my preparation and training as future chemist (36.4%)	Positive and useful for the course (45.4%)	Positive, but not very useful for my training (9.1%)	Neither positive nor negative (0%)	Negative since it is not very useful (0) or negative since it is too complex (0%)

[a]Total number of students who answered the anonymous survey, $n = 22$.

instance, to compare the results obtained by using the *EVOODec* tool applied to several EVOO samples and to write short reports on the proposed activities. Finally, the collective discussions that followed these cooperative works revealed the engagement of students in the topic and the consequent major interest in chemistry lessons. Finally, it is worth noticing that during the COVID-19 pandemic the possibility to have free access to digital tools and other resources was crucial.[29,31,59,60] In this respect, the present simulation tool, completely free and easy-to-use without referring to special software and/or high digital skills, is a concrete help for teachers and students.

■ CONCLUSIONS

In this work, an easy-to-use digital tool for the analysis of UV−vis spectra of olive oils in terms of their main pigments content is reported, which was developed in the frame of a project about the chemistry of olive oils. Details about its use with students, examples of didactic activities, and practical applications with implications with real problems, such as that of food adulterations and that of food quality assessment, are reported here. The flexibility and versatility of the digital tool, which is open, adapt well to different types of high schools. The main learning outcomes from a pilot study with two fifth classes (K−12 level) of a technical institute, and with undergraduate students attending an introductory course of spectroscopy performed partially in person and in distance learning mode, indicate a good engagement of students, a good understanding of the main scientific topics, and a high level of interdisciplinary effect among chemistry, informatics, and mathematics.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.1c01015.

Guide for the acquisition and analysis of UV−vis absorption spectra of oils, guide for the installation and first use of the *EVOODec* simulation tool, and examples of assessment tests and guiding questions for high school students (provided in our experimentations) (PDF, DOCX)

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Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

The authors thank the students of the fifth AC and fifth BC classes of "Chemistry and Materials" course of Technical Institute "C. Cattaneo" San Miniato (Pisa), who participated in the project and the undergraduate students who attended the course "Physical Chemistry and Laboratory" during the last semester (February−May 2021). V. D. thanks all collaborators at the University of Pisa who worked in her team on olive oil research (Mario Cifelli, Donatella Ancora, Francesco Buti, Cristina Lazzerini, Eleonora Borello, Daniele Roncucci, Michela Massa, Maurizio Zandomeneghi) and Andrea Serani for helpful and stimulating discussions concerning olive oil chemistry.

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J. Chem. Educ. 2022, 99, 787−798