Ministry of Science and Higher Education of the Russian Federation
NATIONAL RESEARCH
TOMSK STATE UNIVERSITY (NR TSU)
"Tomsk International Science Program" (TIPS)

APPROVED BY
Head of the Main Educational Program
Dr. of science (phys-math), Associate Professor
_____ I. A. Kurzina
signature
« 08 » июня 2023 .

BACHELOR'S THESIS
STUDY OF PHOTOOXIDATION EFFECT ON EDIBLE OILS WITH VISIBLE AND INFRARED SPECTROSCOPY AND CHEMOMETRIC ANALYSIS

Autonomous educational program
27.03.05 - Tomsk International Science Program
Specialization "Innovatics"

Baitserova Iana Victorovna

Bachelor's Thesis Supervisor
Dr. of science (phys-math), Professor
_____ Y. V. Kistenev
signature
« 08 » июня 2023 .

Written by
student group № 861901
_____ I.V. Baitserova
signature
« 08 » июня 2023 .

Tomsk – 2023

Ministry of Science and Higher Education of the Russian Federation

NATIONAL RESEARCH TOMSK STATE UNIVERSITY (NR TSU)

AEP "Tomsk International Science Program"

APPROVE
MAP Head
Dr. of science (phys-math), Associate Professor
_____ I. A. Kurzina
«25» января 2023.

THE TASK

Regarding the bachelor's final qualification work implementation by a student
Baitserova Iana Victorovna
(student's full name)

In the field of study "Innivatics", Autonomous Educational Program "TISP"

1. The bachelor's final qualification work theme (in English and Russian languages)
STUDY OF PHOTOOXIDATION EFFECT ON EDIBLE OILS WITH VISIBLE AND INFRARED SPECTROSCOPY AND CHEMOMETRIC ANALYSIS/ ИССЛЕДОВАНИЕ ВЛИЯНИЯ ФОТООКИСЛЕНИЯ НА ПИЩЕВЫЕ МАСЛА МЕТОДОМ ВИДИМОЙ И ИНФРАКРАСНОЙ СПЕКТРОСКОПИИ И ХЕМОМЕТРИЧЕСКОГО АНАЛИЗА

2. The deadline for the completion of the task:
а) to academic office – 06. июня 2023.
б) to State Examination Board – 09 июня 2023.

3. Description:
The purpose of this work is to identify the best spectroscopic method for identification of
goals and objectives of the FQW, expected results
photooxidation effect on edible oils using principal component analysis
The expected results: identify the most informative spectroscopic technique coupled with principal component analysis to differentiate oils underwent photooxidation process from ones kept in the darkness

Final qualification work supervisor
Professor, Dr. of science (phys-math)
position, work place
_____ / Ю.В. Кистенев
signature *name*

The task is accepted for execution
25 января 2023
date
Байца / Я.В. Байцерова
signature *name*

ABSTRACT

Bachelor's thesis 90 pages, 10 pictures, 9 tables, 7 appendices.

Key words: Edible oils, Raman spectroscopy, fluorescence spectroscopy, ultraviolet-visible spectroscopy, principal component analysis.

The object of the study is photooxidation effect on edible oils.

The subject of the work is the ability of spectroscopic techniques paired with principal component analysis to identify photooxidation effect on different edible oils.

The purpose of the study is to identify the best spectroscopic technique able to differentiate oils exposed to light from ones kept properly with the help of principle component analysis.

Work results:

1)The measurements were analyzed using principal component analysis;

2)The results were compared using the validation score;

3)The best spectroscopic method for each oil was identified.

Brief description.

Studies of real food shelf life are not often applied in scientific studies, mainly because of the time and budget required for such analyses. However, such studies are very useful for understanding the quality changes that edible oils, including Almond oil, group of olive oils (Olive oil France, Olive oil Poland, olive oil Kenya, EVOO Greek, EVOO Italy), vegetable oils (Fortune oil, Gingerly oil, Mustard delhi oil, Sesame oil), and some other oils (Assam oil, Oelh oil, White bottle oil), undergo during the often very long periods of light exposure in the market. With this in mind, we conducted a study where all the above-mentioned oils underwent the photooxidation effect for a year. Spectroscopic techniques used in the current study, including ultraviolet-visible spectroscopy, fluorescence spectroscopy, and Raman spectroscopy, do not need a special sample preparation, which significantly lower the price and time consumed on the study. Principal component analysis (PCA) is a statistical technique used to reduce the dimensionality of large datasets while preserving as much information as possible, is commonly used for identifying patterns and relationships between variables and provides a better understanding of the data by creating a lower-dimensional representation of the dataset that retains most of the relevant information. This allows comparing these techniques in terms of ability to separate photooxidized samples from those kept properly.

CONTENT

GLOSSARY

EVOO – extra virgin olive oil. High-quality, unrefined olive oil that is made from the fruit of the olive tree.

PC – principal component. Linear combination of the original variables in a dataset that captures the maximum amount of variation in the data.

PCA – principal component analysis. Statistical technique used to reduce the dimensionality of a dataset by identifying the most important patterns or trends in the data through the extraction of principal components.

STD – standard deviation. Statistical measure that quantifies the amount of variation or dispersion in a set of data

UV-Vis spectroscopy – ultraviolet-visible spectroscopy. Type of analytical technique that uses light in the ultraviolet and visible regions of the electromagnetic spectrum to study the electronic transitions of molecules

INTODUCTION

Edible oils are commonly used in food production and are crucial in providing essential nutrients in people's daily diet [1]. However, they are susceptible to oxidative degradation, which can lead to the formation of harmful compounds, such as free radicals and peroxides, that adversely affect the oil's quality, nutritional value, and safety. Therefore, it is important to monitor the extent of oxidation in edible oils to ensure their quality and safety.

Spectroscopic techniques have been extensively used for the detection and monitoring of oxidation in edible oils due to their high sensitivity, rapid analysis time, and non-destructive nature. Among these techniques, UV-Vis spectroscopy, fluorescence spectroscopy, and Raman spectroscopy have shown promising results in detecting and monitoring the photooxidation of edible oils.

UV-Vis spectroscopy has been widely used to monitor the changes in the absorbance spectra of edible oils during photooxidation. Fluorescence spectroscopy has also shown great potential in detecting the changes in the fluorescence signal of edible oils during oxidation. Raman spectroscopy, on the other hand, has been used to detect the changes in the Raman signal of edible oils induced by photooxidation.

In addition, multivariate analysis techniques, such as principal component analysis (PCA), have been used to analyze the spectroscopic data obtained from the different spectroscopic techniques to identify key spectral features that contribute to the differentiation of oils undergoing photooxidation.

This diploma work aims to investigate the ability of UV-Vis spectroscopy, fluorescence spectroscopy, and Raman spectroscopy to differentiate oils underwent photooxidation effect with the use of PCA. The research will review existing literature on the application of spectroscopic techniques in monitoring the photooxidation of edible oils and provide an in-depth analysis of the advantages and limitations of each spectroscopic technique. Furthermore, this research will utilize PCA to analyze the spectroscopic data obtained from different spectroscopic techniques to ascertain which spectroscopic method differs spoiled oils from those kept properly.

Through this research, we hope to contribute to the development of more effective methods for monitoring the photooxidation of edible oils and provide a better understanding of the potential of spectroscopic techniques and PCA in food science research.

1. Background information on photooxidation and its effects on edible oils

Photooxidation is a process that occurs when a substance is exposed to light and oxygen, leading to the formation of free radicals and other reactive oxygen species (ROS) [2]. This process is known to cause significant changes in the chemical composition and physical properties of oils, which can have implications for their shelf life, sensory quality, and nutritional value [3].

Spectroscopic methods are commonly used in food science research to analyze the chemical composition and physical properties of different food components. These methods include ultraviolet (UV-Vis) spectrophotometry, Raman spectroscopy, and fluorescence spectroscopy. UV-Vis spectrophotometry is a technique that measures the absorbance of light by a substance in the ultraviolet and visible regions of the electromagnetic spectrum [4]. Raman spectroscopy is a technique that measures the scattering of light by a sample. Raman spectroscopy is particularly useful for studying the vibrational modes of molecules, and can provide information about the functional groups and chemical bonds present in a sample [5]. Fluorescence spectroscopy measures the emission of light by a substance after excitation by a light source, providing information about the presence of specific compounds or functional groups [6].

Principal component analysis (PCA) is a multivariate statistical technique used to analyze large data sets and identify patterns or relationships between variables [7]. This technique has been used in food science research to analyze spectroscopic data and identify differences between samples based on their chemical composition.

1.1 Brief overview of different spectroscopic methods used for analysis

Ultraviolet-visible spectroscopy.

UV-Vis spectroscopy is a technique used to study the interaction of light with matter in the ultraviolet (UV) and visible (Vis) regions of the electromagnetic spectrum. The basic principle of UV-Vis spectroscopy is based on the Beer-Lambert law [8], which states that the amount of light absorbed by a substance is directly proportional to the concentration of the absorbing species in the sample.

UV-Vis spectroscopy has been used to study the photooxidation of edible oils, which indicated the presence of free radicals and secondary oxidation products [9]. It is a powerful tool for the analysis of edible oils and can provide important insights into the chemical and structural changes that occur during processing, storage, and oxidation.

Fluorescence spectroscopy.

Fluorescence spectroscopy is a technique used to study the interaction of light with matter. It involves an exciting of a sample with light of a certain wavelength, and then measuring the light emitted by the sample as it relaxes back to its ground state. This emitted light, or fluorescence, can provide information about the chemical and structural properties of the sample.

The study of fluorescence characteristics of edible oils subjected to thermal and photo-oxidation processes showed a general reduction of fluorescence intensity, which may result from decomposition of the fluorophores. For photooxidised oils together with qualitative changes different for every oil the analysis showed a decrease of the tocopherol and chlorophyll fluorescence [10], as well as the oxidation of lipids [11]. It is considered to be a powerful tool for the analysis of edible oils and can provide important insights into the chemical and structural changes that occur during storage and oxidation.

Raman spectroscopy.

Raman spectroscopy is a non-destructive technique used to study the vibrational modes of molecules in a sample. It involves shining a laser onto the sample, and then measuring the scattered light that results. This scattered light contains information about the molecular vibrations in the sample and can be used to conduct both qualitative and quantitative analysis.

The basic principle of Raman spectroscopy is based on the Raman effect, which occurs when the laser light interacts with the sample, causing a shift in the energy of the light. This shift in energy is known as Raman scattering, named after its discoverer, Indian physicist Sir C. V. Raman, who first observed it in 1928 [12].

Raman spectroscopy has been used to study the composition and structure of edible oils [13], as well as to monitor the lipid oxidation of oils [14]. It is a powerful tool for the analysis of edible oils and can provide important insights into the chemical and structural changes that occur during storage, and oxidation.

1.2 Statement of the research problem and purpose of the study

The aim of this diploma work is to investigate different spectrophotometry methods in terms of differentiation of edible oils which underwent the photooxidation process from oils ones kept in the darkness. Specifically, UV-Vis spectrophotometry, Raman spectroscopy, and fluorescence spectroscopy were used in the current study. The principal component analysis (PCA)

will be used to identify the ability of spectroscopic techniques to differ oils exposed to light from oils kept in dark conditions.

2 Literature review

2.1 In-depth analysis of existing research on the topic

The photooxidation of edible oils is a complex process that can result in the formation of oxidative products and changes in the chemical and physical properties of the oils, including the development of off-flavors, discoloration, and a decrease in nutritional value. The understanding of the photooxidation process is important for the food industry, as it can help to develop strategies to prevent or minimize the damage caused by light exposure. Spectroscopic techniques have been widely used to study the photooxidation process in edible oils. PCA is a multivariate statistical technique that can be used to analyze spectroscopic data and extract useful information.

UV-Vis spectroscopy.

UV-Vis spectroscopy is a powerful tool that has been widely used to study the photooxidation of edible oils. UV-Vis spectroscopy measures the absorption of light in the UV and visible regions of the electromagnetic spectrum, providing information on the electronic transitions of the molecules in the sample. UV–Vis spectroscopy coupled with chemometrics was used effectively to study the impact of heating on edible oils and determine their acid value. The peak at 370 nm is confirmed to be an indicator of the heated oil [15].

Fluorescence spectroscopy:

Fluorescence spectroscopy is another spectroscopic technique that has been used to study the photooxidation of edible oils. Fluorescence spectroscopy measures the emission of light by molecules that have been excited by light of a certain wavelength, providing information on the structural and chemical changes of the molecules in the sample.

The study of fluorescence signal of light and dark samples of extra virgin olive oil (EVOO) showed the significant lower tocopherol, carotenoid and chlorophyll contents, higher values of triglyceride oligopolymers and contained products of secondary oxidation. Therefore, it was made a conclusion that after only 2 months of exposure to light the oils examined could no longer be considered as extra virgin [16], while the official storage period of EVOO is 2 years. The study of fluorescence characteristics of edible oils subjected to thermal and photooxidation processes showed a general reduction of fluorescence intensity, which may result from decomposition of the fluorophores. The study of the total luminescence spectroscopy proved the ability of the technique to characterize the effect of thermal and photo-oxidation on vegetable oils [17]. For photooxidised

oils together with qualitative changes different for every oil the analysis showed a decrease of the tocopherol and chlorophyll fluorescence [10].

Raman spectroscopy.

Raman spectroscopy is a non-destructive spectroscopic technique that has been used to study the photooxidation of edible oils. Raman spectroscopy measures the scattering of light by molecules in the sample, providing information on the vibrational modes of the molecules.

In the research aimed at the study of the thermal degradation of edible oils surface enhanced Raman spectroscopy was used [18]. The comparative study of Raman and visible spectroscopy in terms of adulteration detection with the use of partial linear square (PLS) analysis [19]. The combination of spectroscopic data with PLS regression allowed quantitative measurement of adulterants in EVOO. Specifically, using a validation set of five samples, the root mean square error (MSE) of prediction was 3.3 and 3.2% for Raman and visible spectroscopy, respectively [20].

Conclusion.

Spectroscopic techniques, such as UV-Vis spectroscopy, fluorescence spectroscopy, and Raman spectroscopy, have been widely used to study the photooxidation of edible oils. These techniques provide valuable information on the chemical and physical changes that occur during the photooxidation process. Moreover, these methods are considered to be relatively inexpensive and do not require special sample preparation. PCA has been used to analyze spectroscopic data and extract useful information. The results of these studies have shown that the changes in the spectroscopic parameters are correlated with the degree of photooxidation, indicating the potential use of spectroscopic techniques for monitoring the photooxidation process in edible oils. The combination of PCA with spectrophotometry methods and different statistical approaches allows to clusterize samples based on their features, differentiate groups of samples from each other with high assurance, and determine degradation effects with a minimum sample preparation. The goal of the present work was to investigate the sensitivity of different spectroscopic techniques (Raman spectroscopy, UV-Vis spectroscopy and fluorescence spectroscopy) on the photooxidation effect of various edible oils with the help of PCA.

2.2 Detailed description of spectroscopic techniques used

Spectroscopic methods are powerful analytical tools that can provide valuable information about the chemical and physical properties of a sample. However, each spectroscopic method has its own advantages and limitations. In this section, we will compare the advantages and limitations

of three commonly used spectroscopic methods: UV-Vis spectroscopy, fluorescence spectroscopy, and Raman spectroscopy.

2.2.1 UV-Vis spectroscopy

UV-Vis spectroscopy is a technique for the analysis of organic and inorganic compounds. This technique is based on the absorption of ultraviolet and visible part of the electromagnetic spectrum by the molecules, which results in the promotion of electrons from the ground state to the excited state. The UV-Vis absorption signal provide information about the electronic structure of a molecule, such as the presence of double bonds, conjugated systems, and functional groups. The UV-Vis spectra are also sensitive to the chemical environment of the molecule, such as solvent polarity, pH, and temperature, which makes this technique useful for studying the stability and reactivity of compounds. The basic principle of UV-Vis spectroscopy is based on the Beer-Lambert law (1), which states that the amount of light absorbed by a substance is directly proportional to the concentration of the absorbing species in the sample.

$$A = \varepsilon c l, \tag{1}$$

where A – absorbance;

ε-molar absorption coefficient [$M^{-1}cm^{-1}$];

c – molar concentration;

l – optical path length.

In UV-Vis spectroscopy, a beam of light with a broad range of wavelengths is passed through a sample. The intensity of the light passing through the sample is measured using a detector, and the data is analyzed to determine the absorbance spectrum of the sample. The schematic illustration is presented in the Figure 1. Absorbance spectrum can provide information on electronic transitions of molecules in the sample, which can be used to study the chemical and structural properties of the sample.

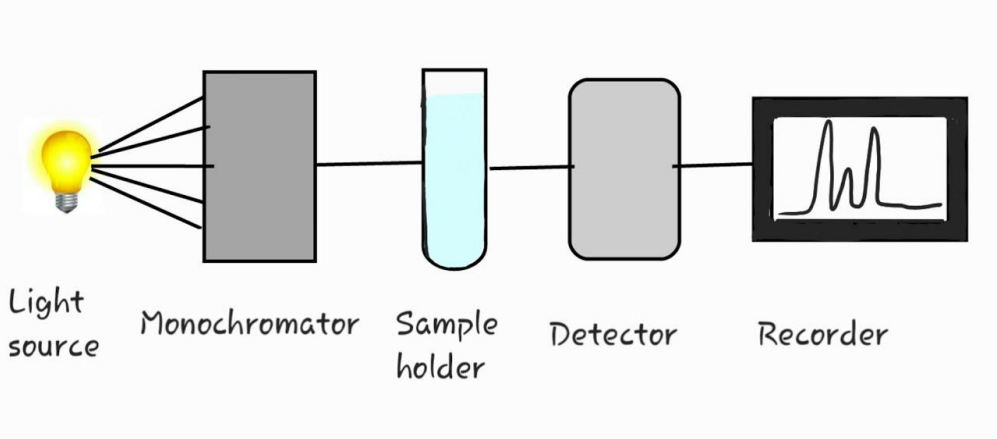


Figure 1 - The schematic representation of the main principle of an UV-Vis spectrometer.

Just like any other spectroscopic technique UV-Vis spectroscopy has its own advantages and limitations. Among advantages the most important are:

- The technique is non destructive, allowing the sample to be reused or proceed to further processing or analyses.
- Measurements can be made quickly, allowing easy integration into experimental protocols.
- Instruments are easy to use, requiring little user training prior to use.
- Data analysis generally requires minimal processing, again meaning little user training is required.
- The instrument is generally inexpensive to acquire and operate, making it accessible for many laboratories [21,22].

However, some of limitations make the technique imperfect. Among them such disadvantages as:

- Stray light. In a real instrument, wavelength selectors are not perfect and a small amount of light from a wide wavelength range may still be transmitted from the light source, possibly causing serious measurement errors. Stray light may also come from the environment or a loosely fitted compartment in the instrument.
- Light scattering. Light scattering is often caused by suspended solids in liquid samples, which may cause serious measurement errors. The presence of bubbles in the cuvette or sample will scatter light, resulting in irreproducible results.

- Interference from multiple absorbing species. A sample may, for example, have multiple types of the green pigment chlorophyll. The different chlorophylls will have overlapping spectra when examined together in the same sample. For a proper quantitative analysis, each chemical species should be separated from the sample and examined individually.

- Geometrical considerations. Misaligned positioning of any one of the instrument's components, especially the cuvette holding the sample, may yield irreproducible and inaccurate results. Therefore, it is important that every component in the instrument is aligned in the same orientation and is placed in the same position for every measurement. Some basic user training is therefore generally recommended to avoid misuse [21,22].

2.2.2 Fluorescence spectroscopy

Fluorescence spectroscopy is a sensitive and selective technique for the analysis of organic and biological samples. Fluorescence spectroscopy is based on the emission of light by the molecules that have been excited by absorption of light. The fluorescence spectra provide information about the electronic structure, energy levels, and molecular environment of the compounds. The basic principle of fluorescence spectroscopy is based on the Jablonski diagram, shown in the Figure 2, which illustrates energy levels of a molecule and transitions that occur during excitation and relaxation. When a molecule absorbs light, it is excited to a higher energy state, and then quickly relaxes back to its ground state by emitting a photon of light. The energy difference between the absorbed and emitted light is characteristic of the molecule and can be used to identify and quantify it.

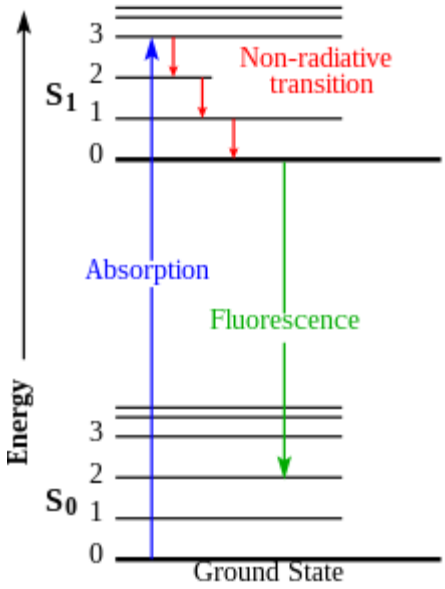


Figure 2 - Jablonski diagram.

Despite all the advantages of fluorescence spectroscopy it has its pros and cons. Among advantages the following can be noted:

- Its high sensitivity is the main advantage of fluorimetry.
- Due to the unique optical properties of the component, it has high specificity.
- You can determine the fluorescence intensity, decay time, and component concentration.
- May be insensitive to light scatter.
- Emitted light is read at the correct angle to the exciting light, reducing background signal
- These types of methods have a wide range of linearity [23].

The limitations of fluorescence spectroscopy include:

- The main disadvantage of fluorescence spectroscopy is that not all molecules fluoresce.
- It has limitations related to loss of recognition ability and photostability.
- Sensitive to interference from changes in sample pH and oxygen levels.

- It is sensitive to sample autofluorescence.
- Problem related to potential toxicity, due to foreign bodies in biological media.
- The short life of fluorophores is another disadvantage of fluorometry [23].

2.2.3 Raman spectroscopy

Raman spectroscopy is a vibrational spectroscopic technique that provides information about molecular structure and chemical bonds of samples. Raman spectroscopy is based on the scattering of light by molecules, which results in a shift in frequency of scattered photons due to interaction with the molecular vibrations. The Raman signal provide information about the functional groups, symmetry, and molecular vibrations of compounds.

In Raman scattering, when a photon interacts with a molecule, the energy of the photon is either absorbed or scattered in a new direction. Most of the scattered light has the same energy as the incident light (which is called Rayleigh scattering), but a small fraction of the scattered light has a different energy due to energy transfer between the molecule and the photon [24]. This shift in energy is known as the Raman shift, and it provides information about the vibrational and rotational modes of the molecule. The scattered light contains a spectrum of frequencies, which corresponds to the vibrational modes of molecules in a sample. A vibrational mode that changes the molecular polarizability (dipole moment induced by the electric field) results in a change in the energy of the incident photon. The difference in energy between incident photons and inelastically scattered photons is called the Raman shift. Graph of the dependence of the intensity of inelastically scattered light on the change in energy is called the Raman spectrum [25].

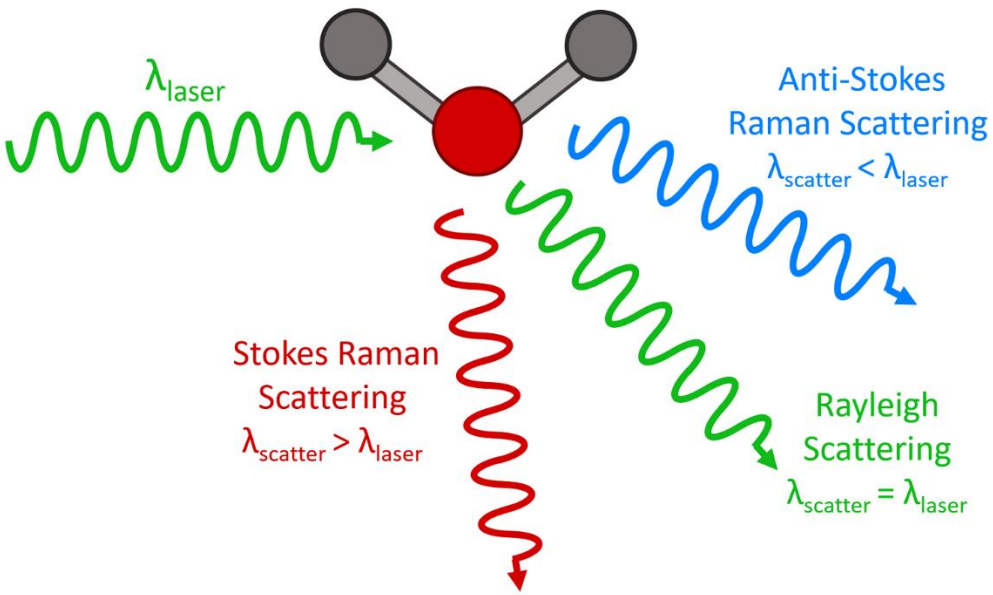


Figure 3 - The schematical representation of the Raman effect.

Despite that fast that Raman spectroscopy is seem to be a promising tool for any kind of studies, it has advantages and disadvantages. The advantages are:

- Many organic and inorganic materials are suitable for Raman analysis. These can be solids, liquids, polymers or vapors.
- No sample preparation needed.
- Not interfered by water.
- Non-destructive.
- Highly specific like a chemical fingerprint of a material.
- Raman spectra are acquired quickly within seconds.
- Samples can be analyzed through glass or a polymer packaging.
- Laser light and Raman scattered light can be transmitted by optical fibers over long distances for remote analysis.
- In Raman spectroscopy, the region from 4000 cm-1 to 50 cm-1 can be covered by a single recording.
- Raman spectra can be collected from a very small volume (< 1 μm in diameter).
- Inorganic materials are easy to analyze with Raman spectroscopy [26].

The disadvantages are:

- Can not be used for metals or alloys.
- The Raman effect is very weak. The detection needs a sensitive and highly optimized instrumentation.
- Fluorescence of impurities or of the sample itself can hide the Raman spectrum. Some compounds fluoresce when irradiated by the laser beam.
- Sample heating through the intense laser radiation can destroy the sample or cover the Raman spectrum [26].

2.2.4 Conclusion

In summary, UV-Vis spectroscopy, Raman spectroscopy, and fluorescence spectroscopy are considered to be powerful tools for the analysis of edible oils and the detection of photooxidation and oxidative degradation products. Each technique has its pros and cons, and the choice of the technique depends on the specific requirements of the analysis. UV-Vis spectroscopy is a versatile and widely used method, but it may not be suitable for the analysis of complex samples. Fluorescence spectroscopy is highly sensitive but can be affected by sample matrix effects. Raman spectroscopy provides highly specific information on the chemical structure and composition of a sample, but its sensitivity can be limited. The combination of these spectroscopic techniques with multivariate analysis, such as principal component analysis (PCA), can provide a more comprehensive and accurate analysis of the samples. Researchers should carefully consider the advantages and limitations of each spectroscopic method when selecting a method for their analysis.

2.3 Machine learning and principal component analysis

Machine learning (ML) is a branch of artificial intelligence that enables computer systems to learn from data and improve their performance on a given task over time. Machine learning (ML) is a field devoted to understanding and building methods that let machines "learn" – that is, methods that leverage data to improve computer performance on some set of tasks [27].

Machine learning algorithms build a model based on sample data, known as training data, in order to make predictions or decisions without being explicitly programmed to do so [28]. Machine learning algorithms are used in a wide variety of applications, such as in medicine, email filtering, speech recognition, agriculture, and computer vision, where it is difficult or unfeasible to develop conventional algorithms to perform the needed tasks [29,30].

A subset of machine learning is closely related to computational statistics, which focuses on making predictions using computers, but not all machine learning is statistical learning. The study of mathematical optimization delivers methods, theory and application domains to the field of machine learning [31].

Machine learning algorithms can be further classified into various categories based on their learning approach [28], such as:

- Supervised Learning. Uses labeled data to train a model to make predictions on new, unseen data.

- Unsupervised Learning. Identifies patterns and relationships within the data itself, without the need for explicit guidance or supervision from a teacher.

- Reinforcement Learning. Learns by interacting with an environment and receiving rewards or penalties based on its actions.

- Semi-supervised Learning. Uses a combination of labeled and unlabeled data to train a model.

Principal Component Analysis (PCA) is an unsupervised learning technique for reducing the dimensionality of high-dimensional data. It involves transforming a set of correlated variables into a new set of uncorrelated variables, known as principal components, while retaining as much of the original variance as possible [32,33].

PCA can be used for a variety of applications, including data visualization, feature selection, and anomaly detection. It can also be used as a preprocessing step prior to using other machine learning techniques such as clustering, classification, or regression [33–37].

Principal component analysis (PCA) is a powerful multivariate data analysis tool that has been widely used in food science research for pattern recognition, data visualization, and data reduction. PCA is a mathematical technique that transforms the original variables in a dataset into a smaller number of uncorrelated variables called principal components (PCs), which capture the most important variations in the data. In this section, we will review the principles and applications of PCA in food science research.

2.3.1 Principles of PCA

PCA is based on the linear algebraic technique of eigenvalue decomposition, which is used to extract the PCs from the original dataset. The first PC is chosen to maximize the variance in the dataset, and each subsequent PC is chosen to maximize the remaining variance in the dataset, subject to the constraint that it is uncorrelated with the previous PCs. The PCs are ordered in decreasing order of variance, and the first few PCs capture most of the variation in the data. The PCs can be plotted in order to visualize the data and identify patterns and relationships among the variables [7].

PCA has many practical applications, such as image compression, noise reduction, feature extraction, and data visualization. In machine learning, PCA is often used as a preprocessing step

to reduce the number of features in a dataset before training a model, which can improve the model's performance and reduce overfitting.

PCA is based on linear algebra and involves several mathematical concepts, including matrix multiplication, eigenvalues, eigenvectors, and singular value decomposition. Here is a brief overview of the mathematical mechanism behind PCA:

- Data standardization is the first step in PCA is to standardize the data by subtracting the mean and dividing by the standard deviation of each variable. This ensures that all variables have the same scale and are centered around zero.

- Covariance matrix. PCA then calculates the covariance matrix of the standardized data. The covariance matrix represents the pairwise correlations between variables in the data.

- Eigenvalues and eigenvectors are the next step. It is aimed at finding the eigenvectors and eigenvalues of the covariance matrix. The eigenvectors are the directions along which the data varies the most, and the corresponding eigenvalues represent the amount of variability along each eigenvector.

- Principal components are the step where the eigenvectors are arranged in descending order of their corresponding eigenvalues to obtain the principal components. The first principal component is the direction that captures the most variability in the data, and each subsequent principal component captures the remaining variability in an orthogonal direction.

- Dimensionality reduction. Finally, PCA projects the data onto the principal components to obtain a lower-dimensional representation of the data. This is achieved by multiplying the standardized data matrix by the matrix of eigenvectors, which results in a new matrix with the same number of rows as the original data but fewer columns corresponding to the chosen number of principal components.

The result is a transformed dataset that retains most of the important information in the original data but with a lower dimensionality. This can be useful for data visualization, feature selection, and other applications where high-dimensional data is a challenge [38–43].

2.4 Applications of PCA in food science research

PCA has been widely used in food science research for a variety of applications, including:

- Sensory analysis. PCA can be used to analyze sensory data from trained panels or consumers, to identify the key sensory attributes that contribute to the overall liking or disliking of a product [44].

- Quality control. PCA can be used to analyze chemical or physical data from food samples, to detect outliers, trends, or differences among samples or batches [45].

- Food authentication. PCA can be used to analyze spectral or chromatographic data from food samples, to identify patterns and markers that can be used for food authentication or traceability [46].

- Nutritional analysis. PCA can be used to analyze nutrient data from food samples, to identify patterns and relationships among the nutrients and the food matrix [47].

PCA has been applied in a wide range of food science research areas, such as food chemistry, food microbiology, food processing, and food sensory analysis. To summarize it can be said, that PCA is a powerful multivariate data analysis tool that has been widely used in food science research for pattern recognition, data visualization, and data reduction. PCA can provide valuable insights into the relationships among the variables in a dataset, and can help to identify patterns and trends that may not be apparent from simple univariate analysis. PCA can be used in a wide range of food science research areas, and can help to improve the understanding of food composition, quality, and sensory attributes.

3 Materials and methods

3.1 Materials

The studied sample consists of 13 oils divided into 2 groups. Oil samples included almond oil, assam oil, extra virgin olive oil (EVOO) Greek, EVOO Italy, fortune oil, oelh oil, olive oil France, olive oil Kenya, olive oil Poland, sesame oil, white oil. One of the groups was kept in darkness (‘dark’). Oils of the second group were kept in the presence of light (‘light’). The study was carried out in order to identify the most informative spectroscopic technique in identifying the photooxidation effect on edible oils with the help of PCA. The samples were investigated by three various optical spectroscopic methods.

3.2 Experimental setup

Different spectroscopic techniques were used in this study to evaluate oils. A portable near-IR Raman spectrometer AvaRaman-785 TEC (Avantes BV, The Netherlands) was used to record and analyze Raman spectra of oils. The system is equipped with a diode laser (wavelength and bandwidth are 785 nm and < 0.2 nm, resolution 7 cm−1 respectively), spectrometer (AvaSpec-ULS2048LTEC, Avantes BV, The Netherlands) with grating (785–1080 nm), Raman probe, and sample holder. The samples were loaded (200 μL in each well) in a 96-well plate (Microplate 96/F, Eppendorf, Germany), and the laser was focused using a Raman probe, placed perpendicular to the plate at a focal length of ~ 1 cm for spectrum acquisition. A Raman spectrum was recorded from the blank wall for the background vibrational spectrum subtraction. The baseline correction, spectral smoothing, and spike removal from the Raman spectrum were performed with Spectragryph spectral analysis software (version 1.2.14). Further, the pre-processed Raman spectrum of oil samples were plotted using OriginPro software (version 2020) (OriginLab Corporation, USA) by considering intensity along Y-axis and wavenumber along X-axis. UV–Vis absorbance and fluorescence spectroscopic measurements were acquired using a Varioskan Flash spectrophotometer (Thermo Scientific, USA). To record the spectrum, samples (200 μL in each well) were loaded in triplicates in a 96-well plate. The absorbance spectra were recorded using the SkanIt™ Software 2.4.3 RE software over the spectral range of 250–700 nm, having a scanning wavelength of step size 2 nm with the bandwidth being 5 nm and measurement time of 100 ms. For fluorescence signal measurements, a series of excitation wavelengths and collect the fluorescence signals respectively. The emission was measured up to 750 nm, with a step size of 2 nm. SkanIt™ Software 2.4.3 RE was used for the spectral acquisition with a measurement time of 100 ms. Each of the samples has 10 replicate readings.

All the measured signals were analyzed with the help of PCA in order to identify which spectrophotometry method can provide the most reliable information about the photooxidation effect. All the PCA results were analyzed using the validation score in order to determine the best separation of light and dark samples in the principal components' (PCs') space. Firstly, the results show that a model that uses only the first component of the transformed space in the calculations shows a significantly better quality than a model that uses all features of the original space with the highest dispersion. That is, under certain conditions, the principal component method can transform the source space so that the first component "absorbs" information that explains the values of the target variable well. Secondly, the quality of a model trained on three components appeared to be less informative compared to model of two components.

3.3 Explanation of the principal component analysis process

Principal Component Analysis (PCA) is a multivariate statistical technique that is used in data analysis to identify patterns and relationships in high-dimensional datasets. PCA works by transforming the original variables into a new set of variables called principal components, which are linear combinations of the original variables that explain the maximum amount of variation in the dataset.

The first principal component (PC1) is the linear combination that explains the largest amount of variation in the dataset, followed by the second principal component (PC2), which explains the second largest amount of variation, and so on. By projecting the original data onto the principal components, PCA reduces the dimensionality of the dataset and allows for easier visualization and interpretation of the data [32,33].

PCA can be used for a variety of applications, such as clustering and classification of samples based on their similarity, identification of outliers, and identification of the most important variables that contribute to the variation in the dataset. The latter is particularly useful in fields such as food science, where it can be used to identify the sensory attributes or chemical components that contribute to the overall quality or acceptability of a food product.

The PCA process involves several steps, including data pre-processing, standardization of data, computation of covariance matrix to identify correlations, Computation of the eigenvectors and eigenvalues of the covariance matrix to identify the PCs, creation of a feature vector to decide the PCs, recasting of the data along the PCs' axes and interpretation of the results [32,34–37,48]. There are also various techniques and software packages available for performing PCA, such as MATLAB, R, and Python.

Step 1. Standardization.

The range of variables is calculated and standardized in this process to analyze the contribution of each variable equally. Calculating the initial variables will helps to categorize the variables that are dominating the other variables of small ranges. In order to transform the variables of the same standard, the following formula is to be used:

$$Z = \frac{x - \mu}{\sigma} \tag{2}$$

where $\mu = \frac{\sum x_i}{n}$ – the mean;

$\sigma = \sqrt{\frac{\sum (x_i - \mu)^2}{n}}$ - standard deviation, where x – value in a data set, n – number of values in a data set.

Step 2. Covariance matrix computation.

A covariance matrix is a $N\ x\ N$ symmetrical matrix that contains the covariances of all possible data sets. In this step it is possible to know how the variables of the given data are varying with the mean value calculated. The covariance matrix of two-dimensional data is, given as follows:

$$CV = \begin{pmatrix} COV\ (x,x) & COV(x,y) \\ COV(y,x) & COV(y,y) \end{pmatrix} \tag{3}$$

where $Covariance = \frac{\sum (x - \mu_x) * (y - \mu_y)}{n}$,

where μ_x – mean of x;

μ_y – mean of y;

n – number of data points.

It is worth mentioning that, the covariance of a number with itself is its variance as $COV\ (x,x) = VAR(x)$.

Step 3. Eigenvectors and eigenvalues.

In order to determine the PCS of variables, it is necessary to define eigen value and eigen vectors for the same. Let A be any square matrix. A non-zero vector v is an eigenvector of A if:

$$Av = \lambda v, \tag{4}$$

for some number λ, called the corresponding eigenvalue.

After the computation of the eigen vector components, we have to define eigen values in descending order (for all variables) and it is a list of principal components.

Step 4. Feature vector.

The eigen values represent the principal components and these components represent the data direction. These PCs form a line of new axes for easier evaluation of data and also the differences between the observations can also be easily monitored.

Step 5. Recast the data along the PCs' axes.

Still no changes made to the original data, only PCs are selected and feature vector is formed. This step aims at the reorientation of data from their original axes to the ones calculated from the PCs. This can be done by the following formula:

$$Final\ data\ set = Standardized\ original\ data\ set * Feature\ vecor \tag{5}$$

3.4 Validation score

For the comparison of PCA performance and ability of different spectroscopic techniques to differentiate between light and dark samples of oils the following validation method was used:

Let's assume that we have a set of points $\{p1, p2, \ldots, pn\}$, where each point pi has coordinates (xi, yi) in two-dimensional space. Then the formula for calculating the average of all pairwise distances between these points will look like this:

$$Avg = \frac{1}{n} * \sum_{i=1}^{n-1} \sum_{j=j+1}^{n} dist(p_i, p_j), \tag{6}$$

where $dist(pi, pj)$ is a function that calculates the distance between the points pi and pj in two-dimensional space.

The formula for calculating the distance between two points in two-dimensional space can be written as follows:

$$dist(p_i, p_j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \quad (7)$$

The average pairwise distance was calculated for points belonging to one group (light or dark) of oils samples. After that, the sum of average distances of two groups was divided into the interclusteral distance:

$$Score = \frac{Avg_{light} + Avg_{dark}}{Centre\ dictance}; \quad (8)$$

where $Centre\ dictance$ - the distance between two centres of clusters in Euclidian dimension;

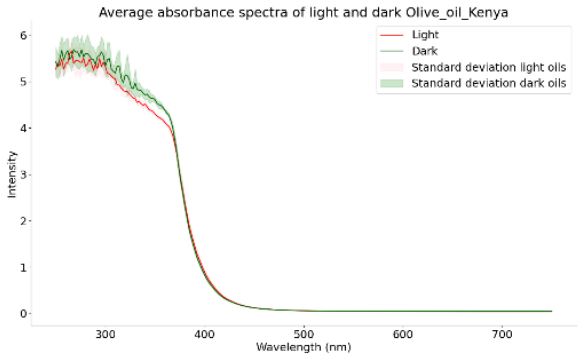
Avg_{light} and Avg_{dark} are the average pairwise distance between cluster's point of light and dark samples respectively.

The probability of intersection of two normal distributions was calculated and appeared to be equal to ~ 0.54 ($\sim 54\%$). In order to do that ~ 770 pairs of normal distributions were created and the probability of their intersection calculated. It is worth mentioning, that the calculations were performed on the data that have no outliers and presents a perfect normal distribution. Therefore, if $Score < 1$ groups are considered to be separated in PCs' space, if $Score = 1$ groups 'touch' each other and can not be defined as separated, if $Score > 1$ groups are not separated in PCs' space. The smaller the Score the better is the separation of oils' groups.

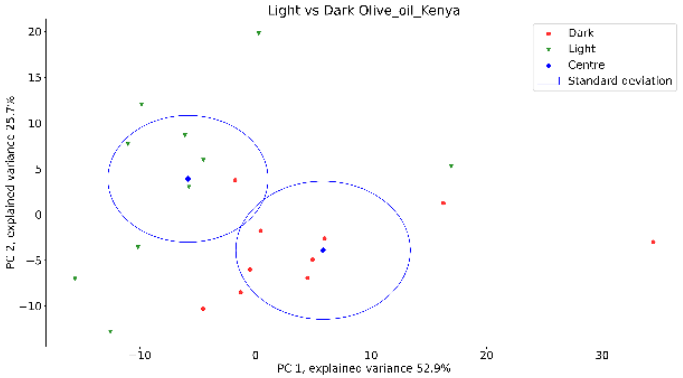
4 Results

4.1 Ultraviolet-visible data

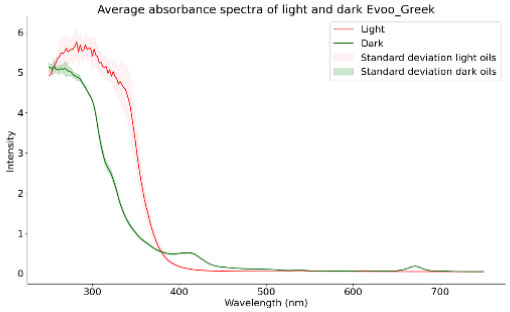
All the samples were investigated using UV-Vis spectroscopy. The average signal of all the studied samples are presented in the Application A together with the PCA results visualization. The most interesting results are shown in the Figure 4. The rest of the analysis's results of UV-Vis spectroscopy samples are presented in the Appendix A. The average signals of Olive oil Kenya light and dark samples are presented in the Figure 4 (a). It can be seen in the figure, that the signal of light and dark samples are very similar to each other and therefore it can be concluded, that there is no possibility to understand which oil was kept properly and which of them was kept in the presence of light. The PCA results are presented in the Figure 4 (d) it can be seen that the standard deviation (STD) of the average distance between all points of clusters and the centres of clusters, presented in the forms of the ovals, overlap with each other. From this it can be concluded, that the samples are not separated in the PCs' space. On the other hand, figure 4 (c) presents the average spectra of EVOO Greek, which can be considered as good example of spectra separation, as light and dark samples have different spectra and could be recognized 'visually'. In the Figure 4 (d) the PCA visualization for EVOO Greek samples is presented. It can be seen, that oil samples are good separated in the PCs' space, as STD of groups do not overlap.



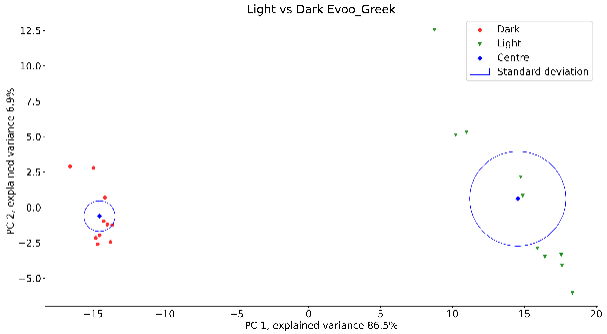
(a)



(b)



(c)



(d)

Figure 4 - The results of analysis of UV-Vis oils data analysis: (a) the average spectra of Olive oil Kenya; (b) the PCA visualization for Olive oil Kenya samples; (c) the average spectra of EVOO Greek; (b) the PCA visualization for EVOO Greek

The validation score was calculated for the results of PCA performance for UV-Vis spectra of oils is presented in the Table 1. From the information presented it can be concluded that the best performance in terms of group separation is shown for EVOO Greek samples, while the worst is shown for Olive oil Kenya, as the validation score is the smallest and the largest respectively. Moreover, the validation score for Olive oil Kenya is greater than 1, and it can be seen in the Figure 4 (b) that STD of clusters' centres overlap, and this sample's groups can not be defined as separated in the PCs' space.

Table 1 - The validation score calculated for all oils absorption samples.

Oil name	Validation score
Almond oil	0,913
Assam oil	0,763
Evoo Greek	0,655
Evoo Italy	0,730
Fortune	0,680
Gingerly oil	0,786
Mustard Delhi	0,672
Oelh	0,980
Olive oil France	0,663
Olive oil Kenya	1,090
Olive oil Poland	0,671
Sesame oil	0,916
White bottle	0,926

4.2 Fluorescence data

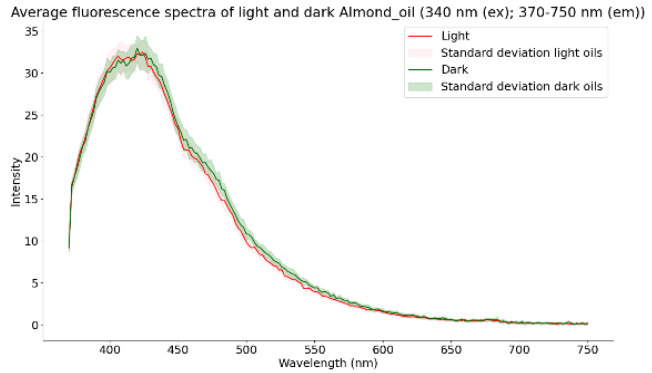
For fluorescence signal measurements a series of excitation and emission wavelengths was investigated. The average fluorescence signal with 340 nm of excitation wavelength and emission wavelength in the range of 370-750 nm of light and dark oil samples are to be discussed in this section. The results of data analysis for Almond oil and EVOO Greek oils are presented in the Figure 5. The rest of the analysis's results of fluorescence spectroscopy (340 nm (ex); 370-750 nm (em)) samples are presented in the Appendix B. The average fluorescence signal of light and dark samples of Almond oil, presented in the Figure 5 (a), are considered to be identical and it is therefore believed, that the groups of oil are impossible to separate taking into the consideration only spectroscopic data. The PCA results visualization for Almond oil groups, presented in the Figure 5 (b), presents that groups are possible to separate in the PCs' space, the centres' STD do not overlap each other. The average fluorescence signal of light and dark sample of EVOO Greek oil, presented in the Figure 5 (c), show absolutely different intensity patterns. The average spectra of dark samples have a peak in the approximate 650-700 nm of excitation wavelength, which can

be a sign of inability of some molecules to luminescence because of long light exposure. The groups are successfully separated in the PCs' space, as can be seen in the Figure 5 (c).

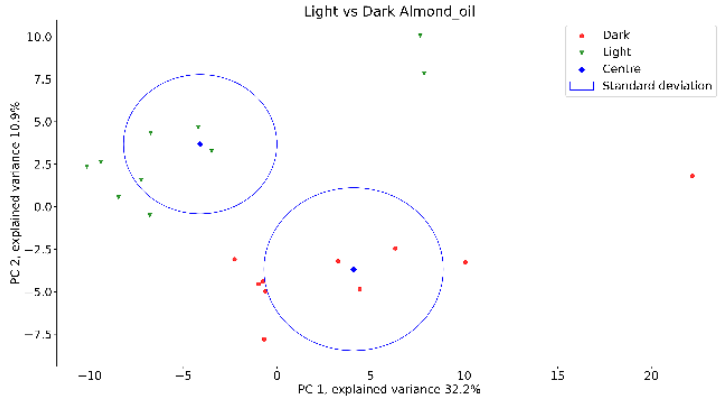
The validation score was calculated for the results of PCA performance for Fluorescence with 340 nm of excitation wavelength spectra of oils is presented in the Table 2. The best performance in terms of group separation the PCs' space is presented for EVOO Greek oils. As the validation score is the smallest among all oils. While the worst separation result is shown for Almond oil samples, as the validation score is the largest among all oils. However, it is worth mentioning, that despite the extreme similarity of groups' spectra for Almond oil samples, the PCA is still able to separate these groups successfully.

Table 2 - The validation score calculated for all fluorescence (340 nm (ex)) results.

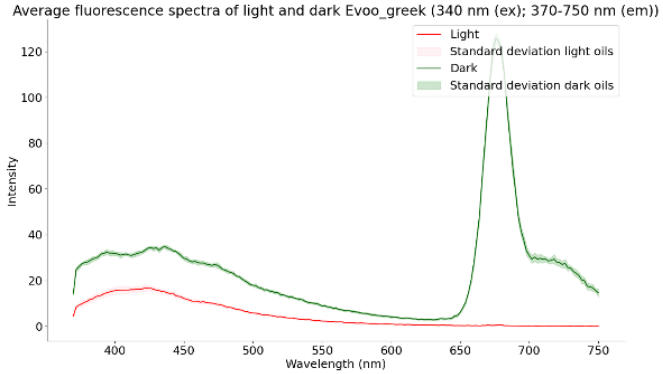
Oil name	Validation score
Almond oil	0,942
Assam oil	0,672
Evoo Greek	0,666
Evoo Italy	0,674
Fortune	0,676
Gingerly oil	0,781
Mustard Delhi	0,667
Oelh	0,940
Olive oil France	0,666
Olive oil Kenya	0,668
Olive oil Poland	0,667
Sesame oil	0,668
White bottle	0,668



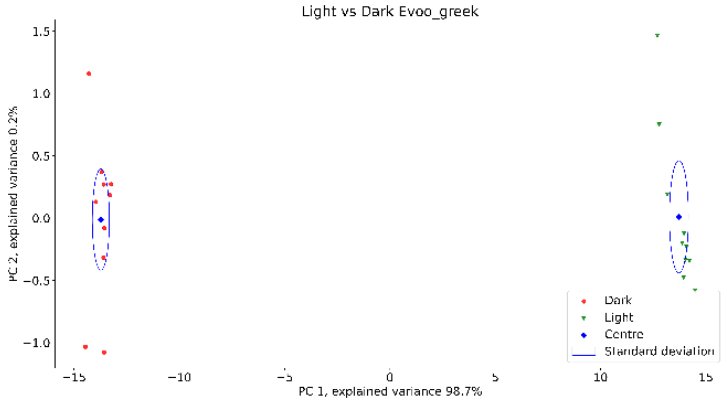
(a)



(b)



(c)



(d)

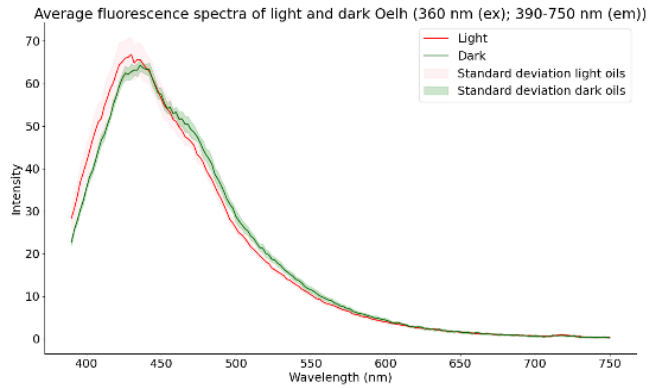
Figure 5 - The results of analysis of Fluorescence (340 nm (ex), 370-750 nm (em)) oils data analysis: (a) the average signal of Almond; (b) the PCA visualization for Almond oil samples; (c) the average signal of EVOO Greek; (b) the PCA visualization for EVOO Greek.

The average fluorescence signal with 360 nm of the excitation wavelength and emission wavelength in the range of 390-750 nm in general show the pattern of light group spectra's flattening. The results of analysis of Oelh and Assam oil are shown in the Figure 6. The rest of the analysis's results of fluorescence spectroscopy (360 nm (ex); 390-750 nm (em)) samples are presented in the Appendix C. From the average signal of light and dark samples of Oelh oil, presented in the Figure 6 (a) it can be seen that their signals are similar to each other and it is considered to be impossible to separate samples of oil kept in the presence of light from oil samples kept properly. Despite this fact PCA visualization, presented in the Figure 6 (b), shows that groups can be separated in the PCs' space. The average signals of two group of Assam oil, Figure 6 (c), show the significant difference. The average signals of light oil group show a higher peak in intensity in the region from 400-450 nm. The groups of the oil samples were successfully separated the PCs' space in the Figure 6 (d).

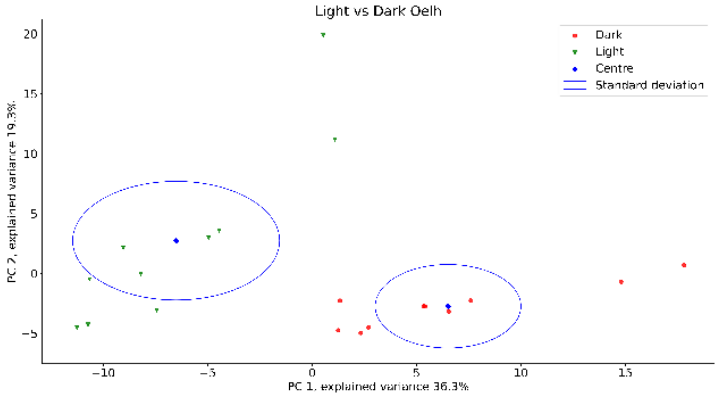
The validation score was calculated for the results of PCA performance for Fluorescence with 360 nm of excitation wavelength spectra of oils is presented in the Table 3. The best performance in terms of group separation the PCs' space is presented for Assam oils. As the validation score is the smallest among all oils. While the worst separation result is shown for Oelh oil samples, as the validation score is the largest among all oils. However, these groups were still well separated from each other in the PCs' space.

Table 3 - The validation score calculated for all fluorescence (360 nm (ex)) results.

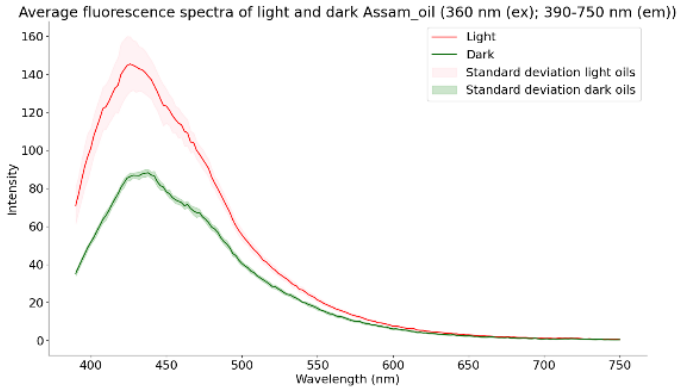
Oil name	Validation score
Almond oil	0,854
Assam oil	0,662
Evoo Greek	0,673
Evoo Italy	0,673
Fortune	0,667
Gingerly oil	0,775
Mustard Delhi	0,667
Oelh	0,873
Olive oil France	0,665
Olive oil Kenya	0,665
Olive oil Poland	0,664
Sesame oil	0,666
White bottle	0,673



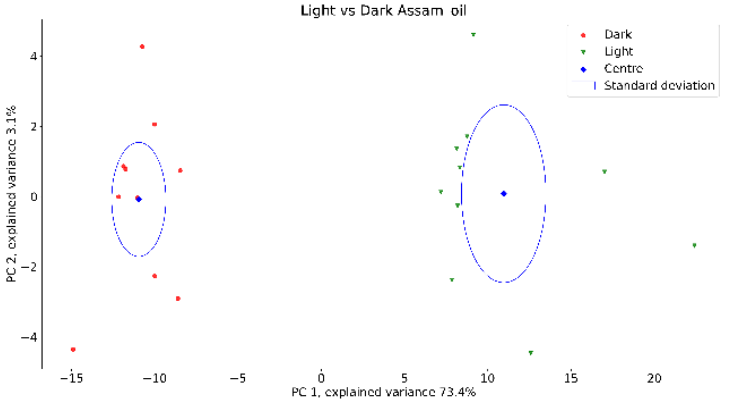
(a)



(b)



(c)



(d)

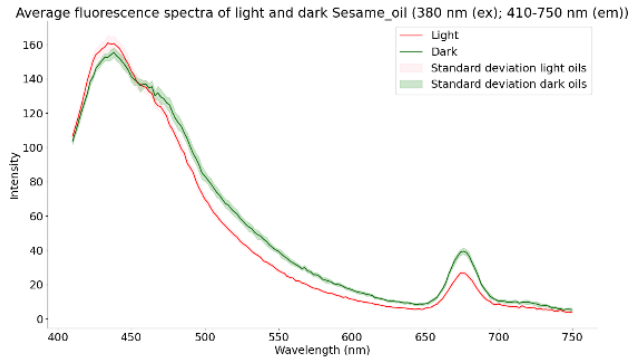
Figure 6 - The results of analysis of Fluorescence (360 nm (ex), 390-750 nm (em)) oils data analysis: (a) the average signal of Oelh oil; (b) the PCA visualization for Oelh oil samples; (c) the average signal of Assam oil; (b) the PCA visualization for Assam oil

The average fluorescence signals with 380 nm of the excitation wavelength and emission wavelength in the range of 410-750 nm in general follows the same pattern of light group spectra flattering. The results of EVOO Italy oil and Sesame oil samples analysis are shown in the Figure 7. The rest of the analysis's results of fluorescence spectroscopy (380 nm (ex); 410-750 nm (em)) samples are presented in the Appendix D. The average signals of light and dark samples of Sesame oil, shown in the Figure 7 (a), repeat each other, meaning, they have peaks in the same regions, with the small difference in intensity. The PCA visualization for Sesame oil groups, presented in the Figure 7 (b), however, shows good separation. For the average signals of EVOO Italy oil, shown in the Figure 7(c), it is an obvious difference of light and dark oil samples. In average dark samples have a distinctive peak in intensity in the region from 650 to 700 nm of excitation wavelength, while the average light samples remain flat. It is worth mentioning that PCA result shows different group distribution, as dark samples are situated more accurate in the PCs' space compared to light samples as can be seen in the Figure 7 (d).

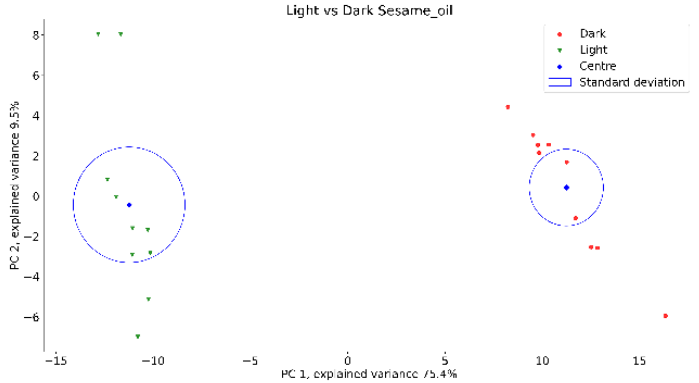
The validation score was calculated for the results of PCA performance for Fluorescence with 380 nm of excitation wavelength spectra of oils is presented in the Table 4. The best performance in terms of group separation the PCs' space is presented for EVOO Italy oil. As the validation score is the smallest among all oils. While the worst separation result is shown for Sesame oil samples, as the validation score is the largest among all oils. However, these groups were still well separated from each other in the PCs' space.

Table 4 - The validation score calculated for all fluorescence (380 nm (ex)) results.

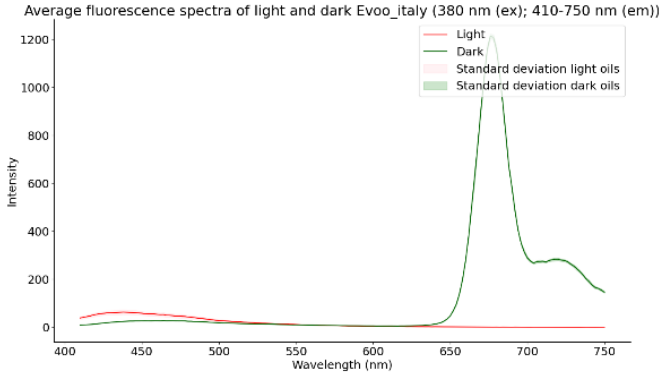
Oil name	Validation score
Almond oil	0,717
Assam oil	0,648
Evoo Greek	0,728
Evoo Italy	0,738
Fortune	0,669
Gingerly oil	0,646
Mustard Delhi	0,657
Oelh	0,704
Olive oil France	0,666
Olive oil Kenya	0,668
Olive oil Poland	0,663
Sesame oil	0,641
White bottle	0,704



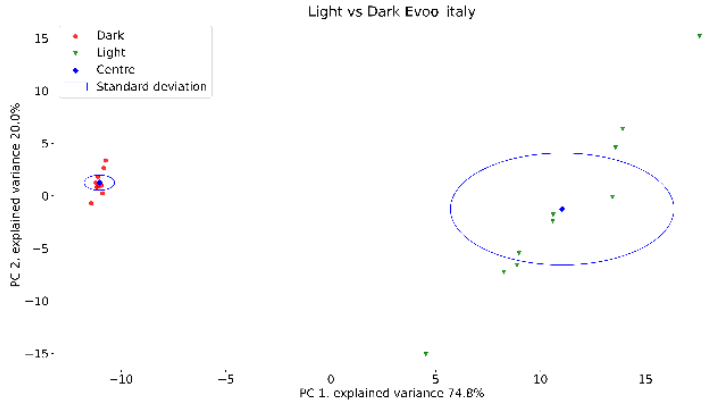
(a)



(b)



(c)



(d)

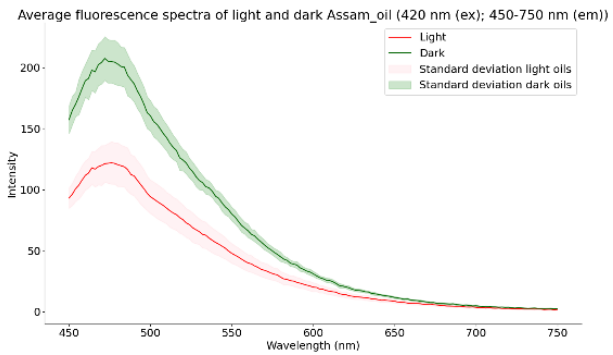
Figure 7 - The results of analysis of Fluorescence (380 nm (ex), 410-750 nm (em)) oils data analysis: (a) the average signal of EVOO Italy oil; (b) the PCA visualization for EVOO Italy samples; (c) the average signal of Sesame oil; (b) the PCA visualization for Sesame oil.

The average fluorescence signals with 420 nm of the excitation wavelength and emission wavelength in the range of 450-750 nm in general continues to follow the same pattern of light group spectra flattering. The result of Assam oil and Fortune oil samples analysis are shown in the Figure 8. The rest of the analysis's results of fluorescence spectroscopy (420 nm (ex); 450-750 nm (em)) samples are presented in the Appendix E. The average signals of light and dark samples of Assam oil, presented in the Figure 8 (a), show identical patterns in terms of peaks with the difference in intensity. The PCA visualization in the Figure 8 (b) shows good separation of light and dark samples. The average signals of dark samples of Fortune oil, shown in the Figure 8 (c), has a peak in the region from 650 to 700 nm, while the light does not have it. The two groups of these oil are separated in the PCs' space in the Figure 8 (d).

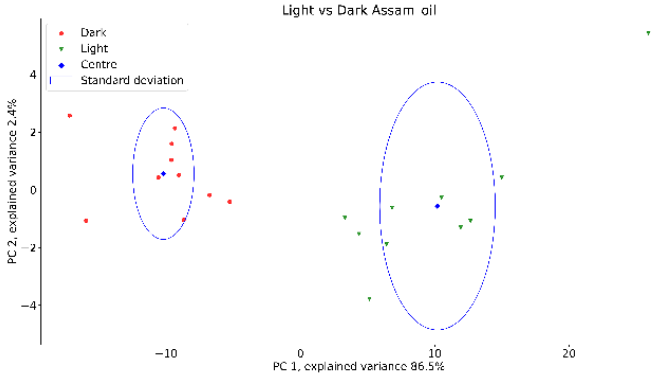
The validation score was calculated for the results of PCA performance for Fluorescence with 420 nm of excitation wavelength spectra of oils is presented in the Table 5. The best performance in terms of group separation the PCs' space is presented for Fortune oil. As the validation score is the smallest among all oils. While the worst separation result is shown for Assam oil samples, as the validation score is the largest among all oils. However, these groups were still well separated from each other in the PCs' space.

Table 5 - The validation score calculated for all fluorescence (420 nm (ex)) results.

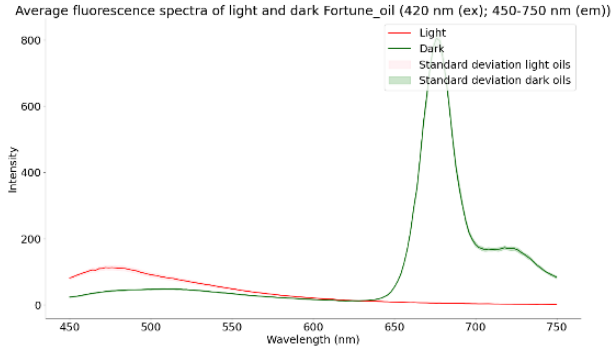
Oil name	Validation score
Almond oil	0,670
Assam oil	0,702
Evoo Greek	0,666
Evoo Italy	0,666
Fortune	0,639
Gingerly oil	0,668
Mustard Delhi	0,675
Oelh	0,666
Olive oil France	0,660
Olive oil Kenya	0,667
Olive oil Poland	0,693
Sesame oil	0,664
White bottle	0,667



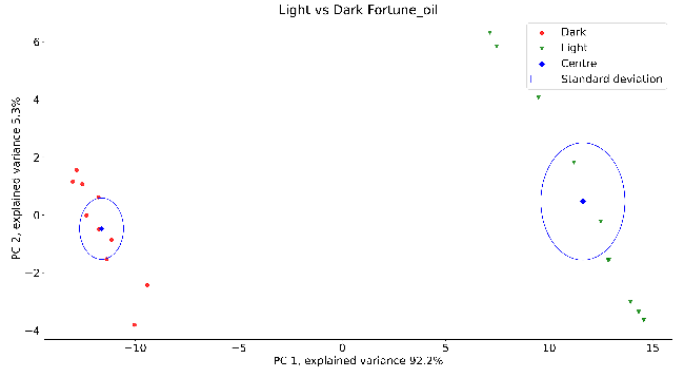
(a)



(b)



(c)



(d)

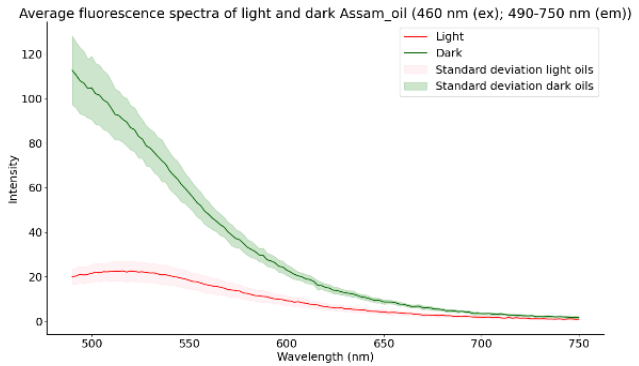
Figure 8 - The results of analysis of Fluorescence (420 nm (ex), 450-750 nm (em)) oils data analysis: (a) the average signals of Assam oil samples; (b) the PCA visualization for Assam oil samples; (c) the average signals of Fortune oil samples; (b) the PCA visualization for Fortune oil.

The average fluorescence signals with 460 nm of the excitation wavelength and emission wavelength in the range of 490-750 nm in general continues to follow the same pattern of light group spectra flattering. The result of Assam oil and Fortune oil samples analysis are shown in the Figure 9. The rest of the analysis's results of fluorescence spectroscopy (460 nm (ex); 490-750 nm (em)) samples are presented in the Appendix F. The average signals of light and dark samples of Assam oil, presented in the Figure 9 (a), show the light samples' signal continues to degrade. The PCA visualization in the Figure 9 (b) shows good separation of light and dark samples. The average signals of dark samples of Fortune oil, shown in the Figure 9 (c), has a peak in the region from 650 to 700 nm, while the light does not have it. The two groups of these oil are separated in the PCs' space in the Figure 9 (d).

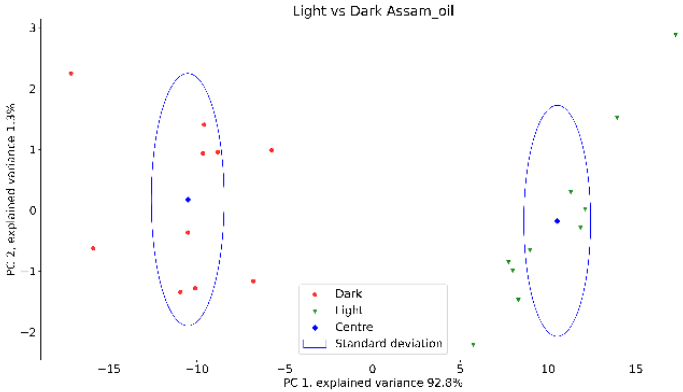
The conclusions made based on the Figure 9 are the same as based on the Figure 8. The validation score was calculated for the results of PCA performance for Fluorescence with 420 nm of excitation wavelength spectra of oils is presented in the Table 6. The best performance in terms of group separation the PCs' space is presented for Fortune oil. As the validation score is the smallest among all oils. While the worst separation result is shown for Assam oil samples, as the validation score is the largest among all oils. However, these groups were still well separated from each other in the PCs' space.

Table 6 - The validation score calculated for all fluorescence (460 nm (ex)) results.

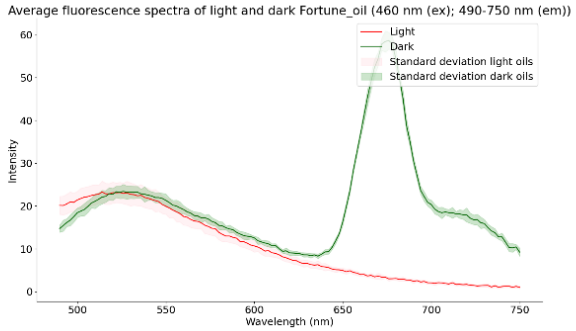
Oil name	Validation score
Almond oil	0,666
Assam oil	0,678
Evoo Greek	0,659
Evoo Italy	0,678
Fortune	0,634
Gingerly oil	0,667
Mustard Delhi	0,672
Oelh	0,674
Olive oil France	0,670
Olive oil Kenya	0,667
Olive oil Poland	0,654
Sesame oil	0,666
White bottle	0,671



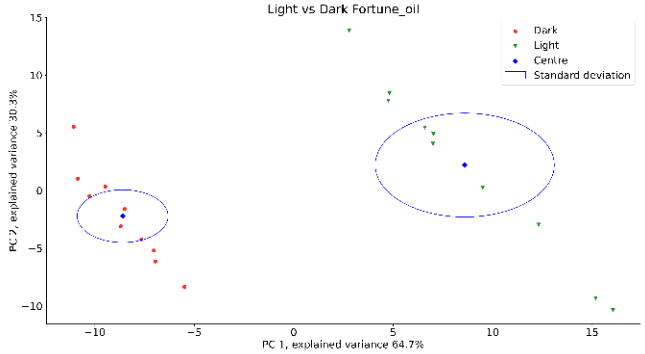
(a)



(b)



(c)



(d)

Figure 9 - The results of analysis of Fluorescence (460 nm (ex), 490-750 nm (em)) oils data analysis: (a) the average signals of Assam oil samples; (b) the PCA visualization for Assam oil samples; (c) the average signals of Fortune oil samples; (b) the PCA visualization for Fortune oil.

Considering everything shown above, it becomes clear that signals of light oils degrade dramatically with the increase in excitation and emission wavelengths in comparison with the spectra of dark oils, which can lead to conclusion that some of molecules either were destroyed by long light exposure or lost ability to luminescence.

Different measurement methods correspond to different PCA performance, however, all of them are considered to be reliable. Nevertheless, the fluorescence data for the highest emission wavelength (460 nm) differs dramatically from the fluorescence data for the lowest wavelength (340 nm).

From this, the conclusion can be made that measurement for the fluorescence with 460 nm of excitation wavelength shows the best data differentiation and therefore, can measure the photooxidation effect with a higher accuracy. It is also worth mentioning that the performance of PCA with data given by fluorescence 460 nm (ex); 490 - 750nm (em) is considered to be more effective in comparison with the PCA performance with data given by fluorescence 340 nm (ex); 370 - 750nm (em), i.e. the validation scores are the smallest for the majority of oils as can be seen in the Table 7.

Table 7 - The validation score calculated for all oils fluorescence samples.

Excitation wavelength (nm)	**340**	**360**	**380**	**420**	**460**
Almond oil	0,942	0,854	0,717	0,670	0,666
Assam oil	0,672	0,662	0,648	0,702	0,678
Evoo Greek	0,666	0,673	0,728	0,666	0,659
Evoo Italy	0,674	0,673	0,738	0,666	0,678
Fortune	0,676	0,667	0,669	0,639	0,634
Gingerly oil	0,781	0,775	0,646	0,668	0,667
Mustard Delhi	0,667	0,667	0,657	0,675	0,672
Oelh	0,940	0,873	0,704	0,666	0,674
Olive oil France	0,666	0,665	0,666	0,667	0,670
Olive oil Kenya	0,668	0,665	0,668	0,660	0,654
Olive oil Poland	0,667	0,664	0,663	0,693	0,667
Sesame oil	0,668	0,666	0,641	0,664	0,666
White bottle	0,668	0,673	0,704	0,667	0,671

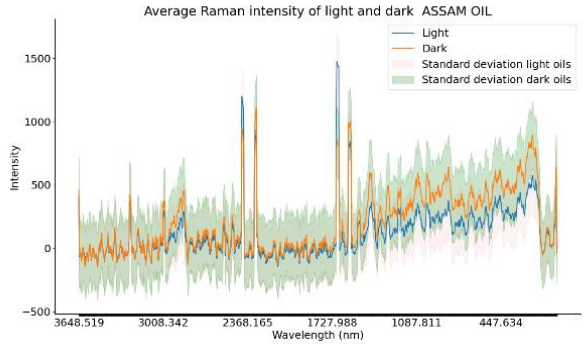
4.3 Raman data

All the samples were investigated using Raman spectroscopy. The average Raman signal for Assam oil and Sesame oil are presented in the Figure 10. The rest of the analysis's results of Raman spectroscopy samples are presented in the Appendix G. Based on the average signals of Assam oil, shown in the Figure 10 (a), it can be said, that the signals of light and dark samples are almost identical as their STD overlap through all the spectra. However, the groups are separated in the PCs' space as can be seen in the Figure 10 (b). It is worth mentioning, that the STD of clusters' centres are situated extremely close to each other, however, they still do not overlap with each other. The average signals of light and dark groups of Sesame oil, presented in the Figure 10 (c), also overlap each other, however have some difference. The PCA visualization in the Figure 10 (d) seem to be a better performance as the groups are situated further away from each other.

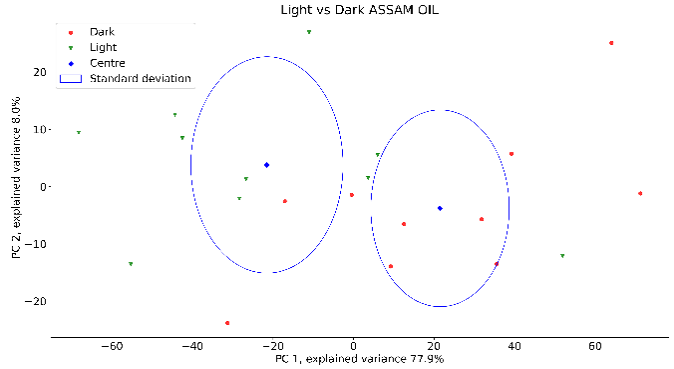
In the Table 8 the validation scores for Raman samples are presented. The best performance in terms of group separation the PCs' space is presented for Sesame oil. As the validation score is the smallest among all oils. While the worst separation result is shown for Assam oil samples, as the validation score is the largest among all oils. It is also worth mentioning, that the validation score calculated for Assam oil groups is significantly close to 1, meaning, the groups are located extremely close to each other. However, these groups were still well separated from each other in the PCs' space.

Table 8 - The validation score calculated for all Raman samples.

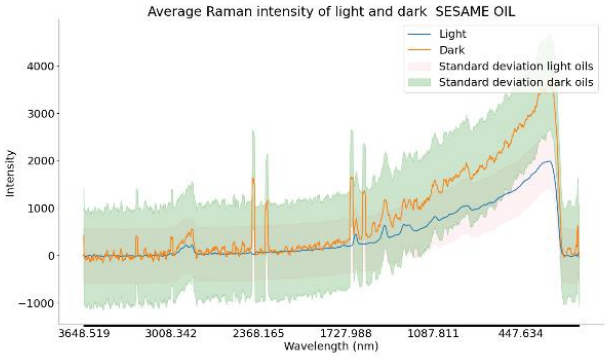
Oil name	Validation score
Almond oil	0,689
Assam oil	0,989
Evoo Greek	0,678
Evoo Italy	0,690
Fortune	0,694
Gingerly oil	0,734
Mustard Delhi	0,673
Oelh	0,723
Olive oil France	0,719
Olive oil Kenya	0,832
Olive oil Poland	0,695
Sesame oil	0,667
White bottle	0,684



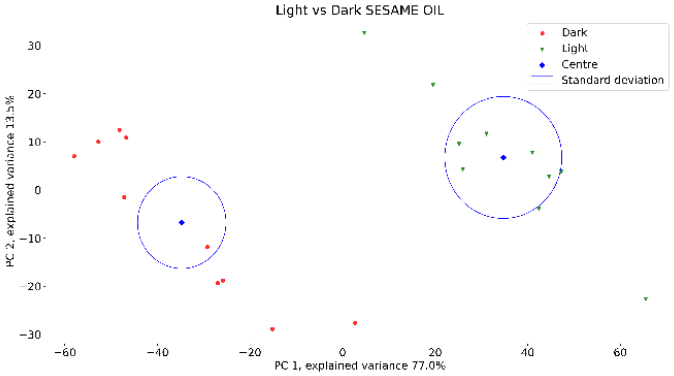
(a)



(b)



(c)



(d)

Figure 10 - The results of analysis of Raman oils data analysis: (a) the average signals of Assam oil samples; (b) the PCA visualization for Assam oil samples; (c) the average signals of Sesame oil samples; (b) the PCA visualization for Sesame oil.

4.4 Comparison of all spectroscopic techniques coupled with PCA

In order to determine the most informative spectroscopic method in combination with PCA it makes sense to compare the validation scores calculated for all PCA results in the Table 9.

Table 9 - The validation score for all PCA results.

	Fluorescence excitation wavelength (nm)							
Oil name	**340**	**360**	**380**	**420**	**460**	**UV-Vis**	**Raman**	**Min**
Almond oil	0,942	0,854	0,717	0,670	0,666	0,913	0,689	0,666
Assam oil	0,672	0,662	0,648	0,702	0,678	0,763	0,989	0,648
Evoo Greek	0,666	0,673	0,728	0,666	0,659	0,655	0,678	0,655
Evoo Italy	0,674	0,673	0,738	0,666	0,678	0,730	0,690	0,666
Fortune	0,676	0,667	0,669	0,639	0,634	0,680	0,694	0,634
Gingerly oil	0,781	0,775	0,646	0,668	0,667	0,786	0,734	0,646
Mustard Delhi	0,667	0,667	0,657	0,675	0,672	0,672	0,673	0,657
Oelh	0,940	0,873	0,704	0,666	0,674	0,980	0,723	0,666
Olive oil France	0,666	0,665	0,666	0,667	0,670	0,663	0,719	0,663
Olive oil Kenya	0,668	0,665	0,668	0,660	0,654	1,090	0,832	0,654
Olive oil Poland	0,667	0,664	0,663	0,693	0,667	0,671	0,695	0,663
Sesame oil	0,668	0,666	0,641	0,664	0,666	0,916	0,667	0,641
White bottle	0,668	0,673	0,704	0,667	0,671	0,926	0,684	0,667

As there is no universal spectroscopic method for all the oils that shows the minimum validation score for all the oils, every oil has its own optimal technique coupled with PCA. Therefore, for Assam oil, Gingerly oil, Mustard Delhi oil, Olive oil Poland, Sesame oil the best spectroscopic technique coupled with PCA appeared to be Fluorescence with 380 nm of excitation wavelength. For EVOO Italy oil, Oelh oil and White bottle oil Fluorescence with excitation wavelength of 420 nm showed the best result of separation in the PCs' space. Fluorescence with 460 nm of excitation appeared to be the best spectroscopic method for Almond oil, Fortune oil and Olive oil Kenya. Only for two oils UV-Vis spectroscopy showed the best separation compared with all other techniques, for EVOO Greek and Olive oil France. Raman spectroscopy together with Fluorescence with 340 and 360 nm of excitation wavelength did not show any significant results and therefore, considered to be the least informative spectroscopic methods coupled with PCA in the studies of photooxidation effect of edible oils.

5. Conclusion

The current work investigated the ability of different spectroscopic techniques coupled with PCA to identify the photooxidation effect on edible oils. Different spectroscopic techniques were used in order to identify the best method for identifying the photooxidation effect on edible oils. During the work 2 groups of 13 edible oils were investigated with the help of UV-Vis spectroscopy, fluorescence spectroscopy and Raman spectroscopy. The groups included light samples (oils that were kept in the presence of light for 1 year) and dark samples (oils kept in the darkness). The spectra of samples were analyzed with the help of PCA and the division of two groups of oils in PCs' space were analyzed using validation score, presenting the relation of sum of average distances of samples inside the clusters to the distance between centres of two clusters.

As the result of the work, it can be stated that UV-Vis spectroscopy and fluorescence spectroscopy coupled with PCA showed good sample separation, however, the Raman spectra did not show any significant results to be considered the best method to identify photooxidation effect for any of the investigated oils.

It is worth mentioning that such unsupervised machine learning technique as PCA is appeared to be good tool for identifying photooxidized oils, as it separated all the samples despite the spectroscopic method.

REFERENCES

1. Frankel E.N. Antioxidants in lipid foods and their impact on food quality // Food Chem. Elsevier, 1996. Vol. 57, № 1. P. 51–55.

2. Frankel E.N. Lipid oxidation: Mechanisms, products and biological significance // J. Am. Oil Chem. Soc. John Wiley & Sons, Ltd, 1984. Vol. 61, № 12. P. 1908–1917.

3. Martínez S., Carballo J. Physicochemical, Sensory and Nutritional Properties of Foods Affected by Processing and Storage // Foods. Multidisciplinary Digital Publishing Institute (MDPI), 2021. Vol. 10, № 12.

4. Spectroscopic Methods in Food Analysis - Google Books [Electronic resource]. URL: https://books.google.ru/books?hl=en&lr=&id=SmpQDwAAQBAJ&oi=fnd&pg=PP1&dq=Spectroscopic+methods+in+food+analysis.+&ots=rtB7yGWdgr&sig=Ix9Cv05n8JKj2EMMDUA9nGMKscs&redir_esc=y#v=onepage&q=Spectroscopic methods in food analysis.&f=false (accessed: 24.03.2023).

5. Winefordner E.J.D. Frontmatter // Raman Spectrosc. Chem. Anal. John Wiley & Sons, Ltd, 2005. P. i–xxiv.

6. Wang T. et al. Rapid identification and quantification of cheaper vegetable oil adulteration in camellia oil by using excitation-emission matrix fluorescence spectroscopy combined with chemometrics // Food Chem. Elsevier, 2019. Vol. 293. P. 348–357.

7. Jollife I.T., Cadima J. Principal component analysis: a review and recent developments // Philos. Trans. R. Soc. A Math. Phys. Eng. Sci. The Royal Society Publishing, 2016. Vol. 374, № 2065.

8. Ultraviolet-Visible (UV-Vis) Spectroscopy – Derivation of Beer-Lambert Law | Analytical Chemistry | PharmaXChange.info [Electronic resource]. URL: https://pharmaxchange.info/2012/04/ultraviolet-visible-uv-vis-spectroscopy-–-derivation-of-beer-lambert-law/ (accessed: 29.04.2023).

9. Rabiej D., Szydłowska-Czerniak A. Fluorescence and UV-VIS Spectroscopy to Determine the Quality Changes of Rapeseed Oil Fortified with New Antioxidant After Storage Under Various Conditions // Food Anal. Methods. Springer, 2020. Vol. 13, № 10. P. 1973–1982.

10. Sikorska E. et al. Characterization of edible oils using total luminescence spectroscopy // J. Fluoresc. Kluwer Academic/Plenum Publishers, 2004. Vol. 14, № 1. P. 25–35.

11. Choe E., Min D.B. Chemistry of Deep-Fat Frying Oils // J. Food Sci. John Wiley & Sons, Ltd, 2007. Vol. 72, № 5. P. R77–R86.

12. Raman C. V. A new radiation // Proc. Indian Acad. Sci. - Sect. A. Springer, 1953. Vol. 37, № 3. P. 333–341.

13. Jin H. et al. Application of Raman spectroscopy in the rapid detection of waste cooking oil // Food Chem. Elsevier, 2021. Vol. 362. P. 130191.

14. Muik B. et al. Direct monitoring of lipid oxidation in edible oils by Fourier transform Raman spectroscopy // Chem. Phys. Lipids. Elsevier, 2005. Vol. 134, № 2. P. 173–182.

15. Zhang W. et al. A unique quantitative method of acid value of edible oils and studying the impact of heating on edible oils by UV–Vis spectrometry // Food Chem. Elsevier, 2015. Vol. 185. P. 326–332.

16. Baltazar P. et al. Development of Rapid Extra Virgin Olive Oil Quality Assessment Procedures Based on Spectroscopic Techniques // Agron. 2020, Vol. 10, Page 41. Multidisciplinary Digital Publishing Institute, 2019. Vol. 10, № 1. P. 41.

17. Sikorska E. et al. Characterization of edible oils using total luminescence spectroscopy // J. Fluoresc. Kluwer Academic/Plenum Publishers, 2004. Vol. 14, № 1. P. 25–35.

18. Lam H.Y., Roy P.K., Chattopadhyay S. Thermal degradation in edible oils by surface enhanced Raman spectroscopy calibrated with iodine values // Vib. Spectrosc. Elsevier, 2020. Vol. 106. P. 103018.

19. Philippidis A. et al. Comparative Study using Raman and Visible Spectroscopy of Cretan Extra Virgin Olive Oil Adulteration with Sunflower Oil // http://dx.doi.org/10.1080/00032719.2016.1208212. Taylor & Francis, 2017. Vol. 50, № 7. P. 1182–1195.

20. Drakopoulou S. et al. Comparative Evaluation of Different Targeted and Untargeted Analytical Approaches to Assess Greek Extra Virgin Olive Oil Quality and Authentication // Molecules. 2022. Vol. 27, № 4. P. 1350.

21. Bosch Ojeda C., Sanchez Rojas F. Recent applications in derivative ultraviolet/visible

absorption spectrophotometry: 2009-2011. A review // Microchem. J. 2013. Vol. 106. P. 1–16.

22. Sharpe M.R. Instrumentation: Stray Light in UV-VIS Spectrophotonmeters // Anal. Chem. 1984. Vol. 56, № 2. P. 339A-356A.

23. Advantages and disadvantages of fluorescence spectroscopy [Electronic resource]. URL: https://whatishplc.com/chemistry/advantages-and-disadvantages-of-fluorescence-spectroscopy/ (accessed: 25.03.2023).

24. Smith E., Dent G. Modern Raman spectroscopy : a practical approach. J. Wiley, 2005. P. 210.

25. Long D.A. The Raman Effect: A Unified Treatment of the Theory of Raman Scattering by Molecules. 2002. 610 p.

26. Advantages and disadvantages of Raman Spectroscopy - Romanian Database of Raman Spectroscopy [Electronic resource]. URL: http://www.rdrs.ro/blog/articles/advantages-disadvantages-raman-spectroscopy/ (accessed: 25.03.2023).

27. Mitchell T.M. CHAPTER 1 GENERATIVE AND DISCRIMINATIVE CLASSIFIERS : NAIVE BAYES AND LOGISTIC REGRESSION Learning Classifiers based on Bayes Rule // Mach. Learn. Machine Learning V2, 2010. Vol. 1, № Pt 1-2. P. 1–17.

28. Alpaydin Ethem. Introduction to Machine Learning. 3rd ed. Massachusetts Institute of Technology, 2020.

29. Yoosefzadeh-Najafabadi M. et al. Application of Machine Learning Algorithms in Plant Breeding: Predicting Yield From Hyperspectral Reflectance in Soybean // Front. Plant Sci. Frontiers Media S.A., 2021. Vol. 11.

30. Hu J. et al. Voronoi-Based Multi-Robot Autonomous Exploration in Unknown Environments via Deep Reinforcement Learning // IEEE Trans. Veh. Technol. Institute of Electrical and Electronics Engineers Inc., 2020. Vol. 69, № 12. P. 14413–14423.

31. Ngọc A.V. Data Mining and Statistics: What’s the Connection.

32. Jolliffe I. Principal Component Analysis // Int. Encycl. Stat. Sci. Berlin, Heidelberg: Springer, Berlin, Heidelberg, 2011. P. 1094–1096.

33. Wold S., Esbensen K., Geladi P. Principal component analysis // Chemom. Intell. Lab. Syst. Elsevier, 1987. Vol. 2, № 1–3. P. 37–52.

34. Hastie T., Tibshirani R., Friedman J. High-Dimensional Problems: p N. 2009. P. 649–698.

35. Hastie T., Tibshirani R., Friedman J. Linear Methods for Classification. 2009. P. 101–137.

36. Shlens J. A Tutorial on Principal Component Analysis. 2014.

37. Zhang T., Ramakrishnan R., Livny M. BIRCH. Association for Computing Machinery (ACM), 1996. P. 103–114.

38. Kurita T. Principal component analysis (PCA) // Comput. Vis. A Ref. Guid. 2019. P. 1--4.

39. Jollife I.T., Cadima J. Principal component analysis: a review and recent developments // Philos. Trans. R. Soc. A Math. Phys. Eng. Sci. The Royal Society Publishing, 2016. Vol. 374, № 2065.

40. Salem N., Hussein S. Data dimensional reduction and principal components analysis // Procedia Comput. Sci. Elsevier B.V., 2019. Vol. 163. P. 292–299.

41. Groth D. et al. Principal components analysis // Methods Mol. Biol. Methods Mol Biol, 2013. Vol. 930. P. 527–547.

42. Gewers F.L. et al. Principal Component Analysis: A Natural Approach to Data Exploration // ACM Comput. Surv. Association for Computing Machinery, 2018. Vol. 54, № 4.

43. Mahmoudi M.R. et al. Principal component analysis to study the relations between the spread rates of COVID-19 in high risks countries // Alexandria Eng. J. Elsevier, 2021. Vol. 60, № 1. P. 457–464.

44. Greenhoff K., MacFie H.J.H. Preference mapping in practice // Meas. Food Prefer. Springer US, 1994. P. 137–166.

45. Gene-expression Profiling in Non-small Cell Lung Cancer with Invasion of Mediastinal Lymph Nodes for Prognosis Evaluation [Electronic resource]. URL: https://www.researchgate.net/publication/282343896_Gene-expression_Profiling_in_Non-small_Cell_Lung_Cancer_with_Invasion_of_Mediastinal_Lymph_Nodes_for_Prognosis_

Evaluation (accessed: 25.03.2023).

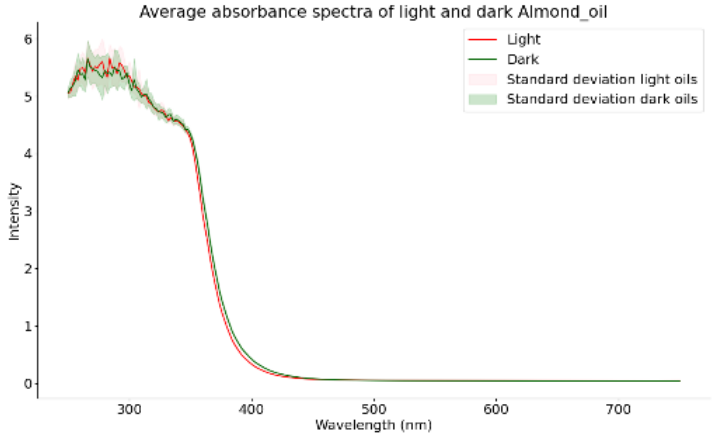
46. Tsimidou M., Macrae R., Wilson I. Authentication of virgin olive oils using principal component analysis of triglyceride and fatty acid profiles: Part 2—Detection of adulteration with other vegetable oils // Food Chem. Elsevier, 1987. Vol. 25, № 4. P. 251–258.

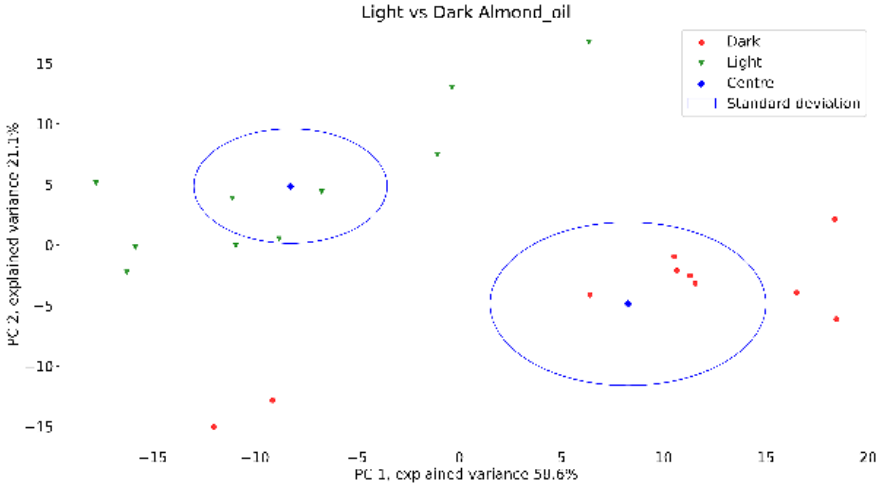
47. Smith A.D.A.C. et al. Dietary patterns obtained through principal components analysis: the effect of input variable quantification // Br. J. Nutr. Br J Nutr, 2013. Vol. 109, № 10. P. 1881–1891.

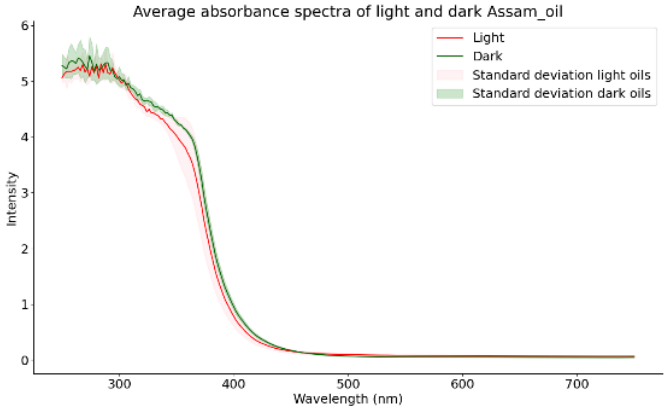
48. Hastie T., Tibshirani R., Friedman J. The Elements of Statistical Learning. New York, NY: Springer New York, 2009.

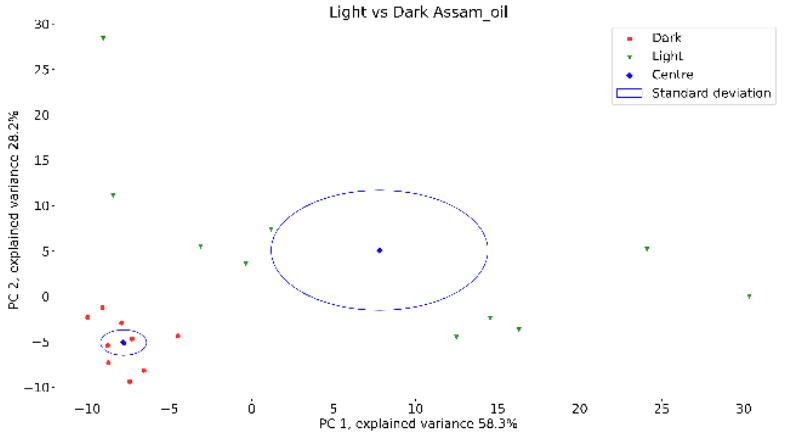
APPENDIX A.

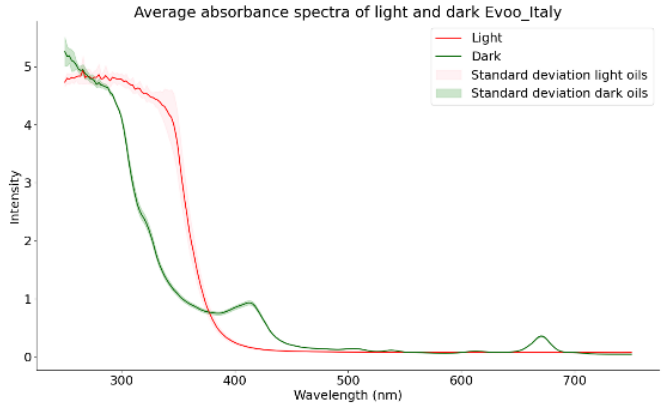
Figure A.1 - The results of analysis UV-Vis spectroscopy oils analysis and PCA visualization.

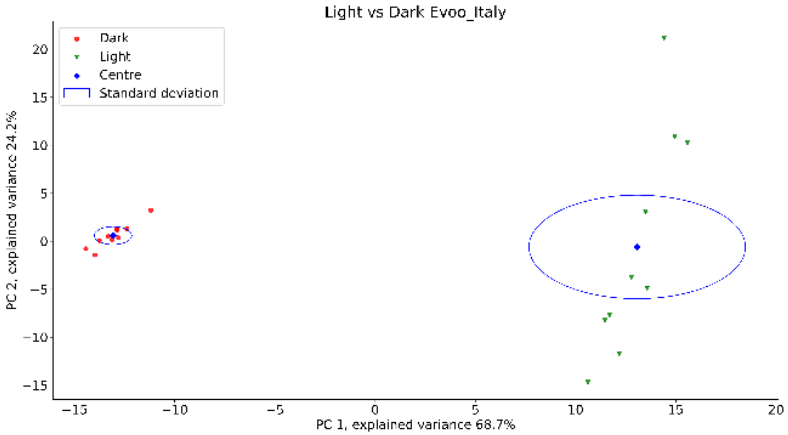


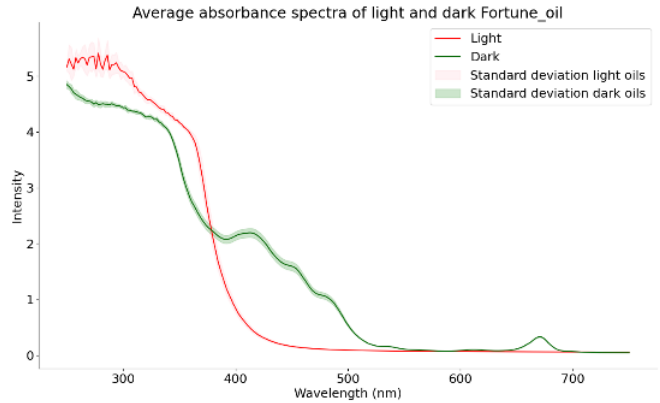


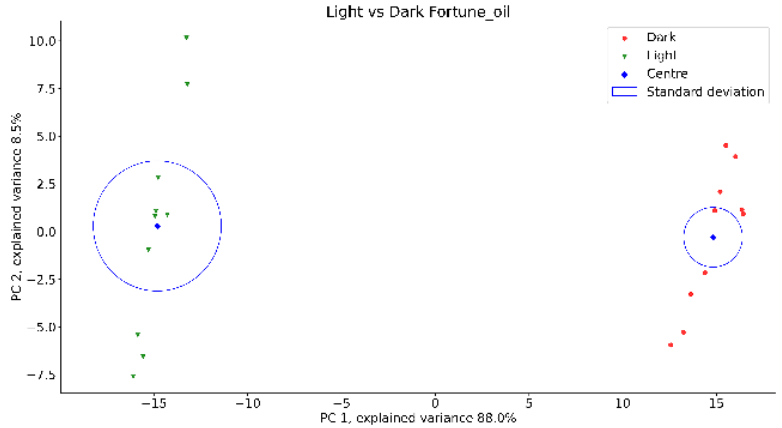

Average absorbance spectra of light and dark Assam_oil
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

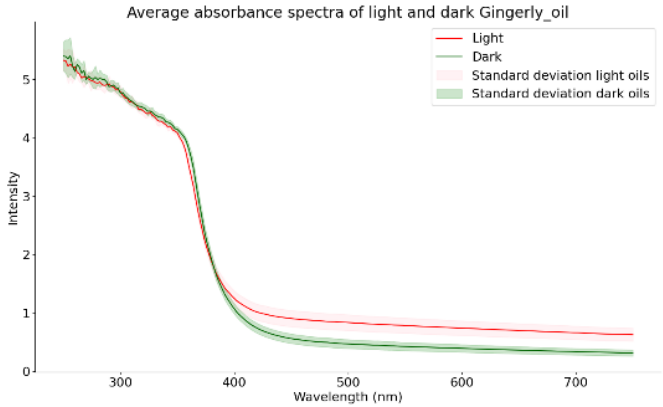

Light vs Dark Assam_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 28.2%
PC 1, explained variance 58.3%

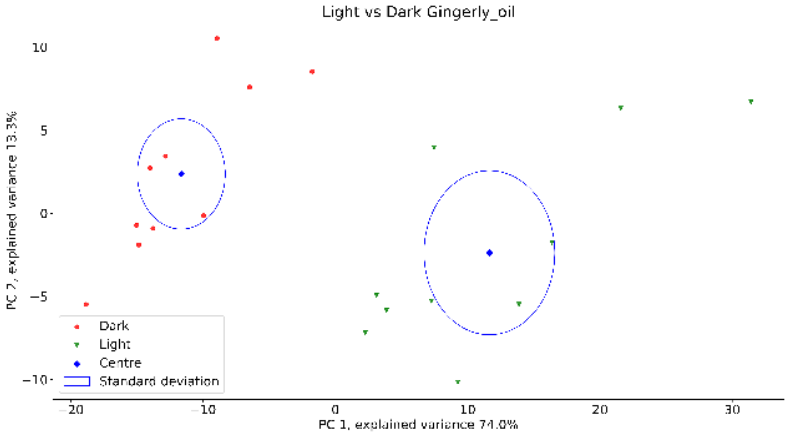

Average absorbance spectra of light and dark Evoo_Italy
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

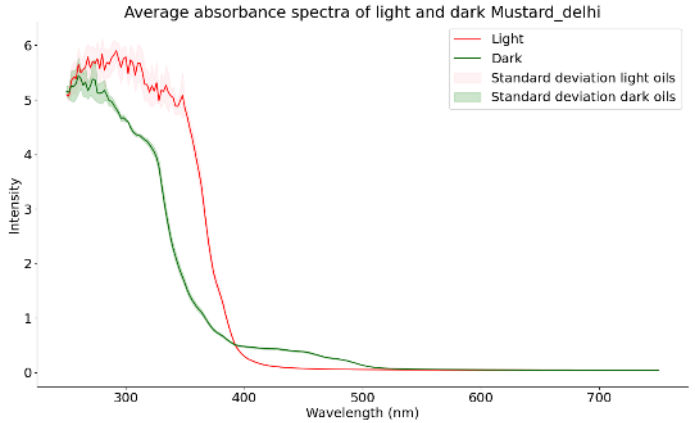

Light vs Dark Evoo_Italy
Dark
Light
Centre
Standard deviation
PC 2, explained variance 24.2%
PC 1, explained variance 68.7%

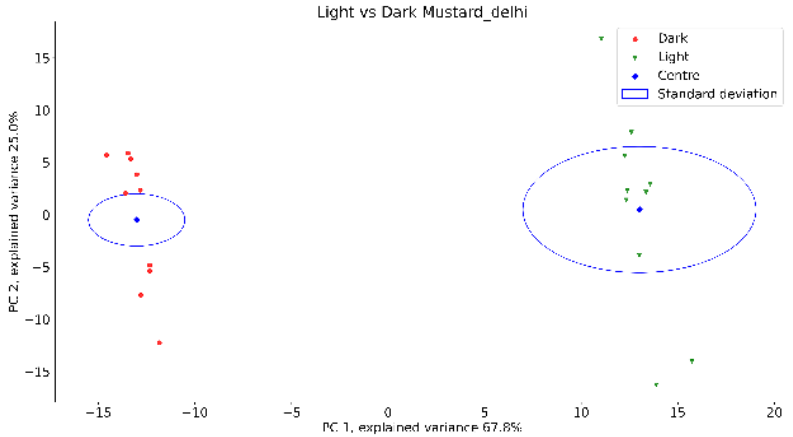

Average absorbance spectra of light and dark Fortune_oil
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

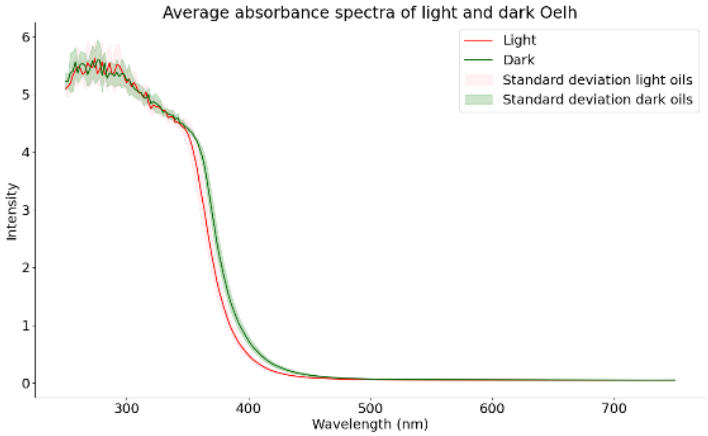

Light vs Dark Fortune_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 8.5%
PC 1, explained variance 88.0%

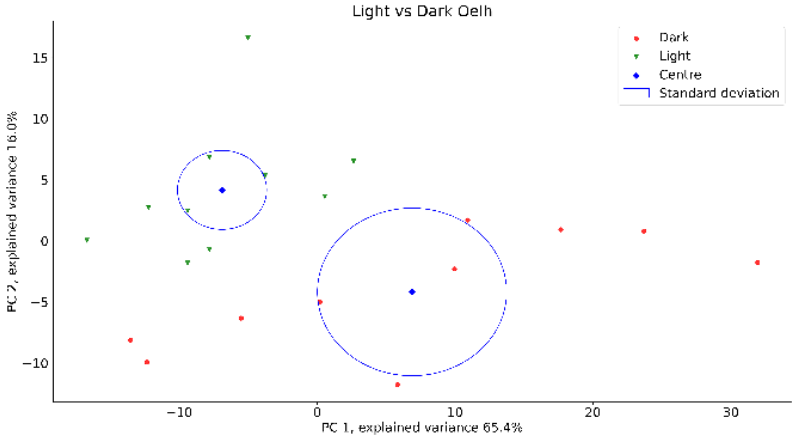

Average absorbance spectra of light and dark Gingerly_oil
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

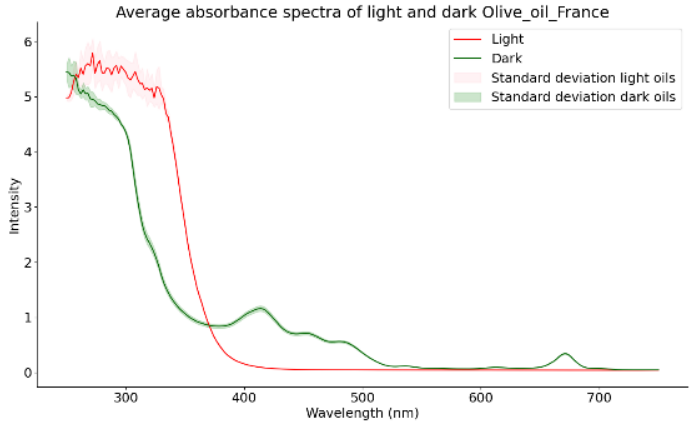

Light vs Dark Gingerly_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 13.3%
PC 1, explained variance 74.0%

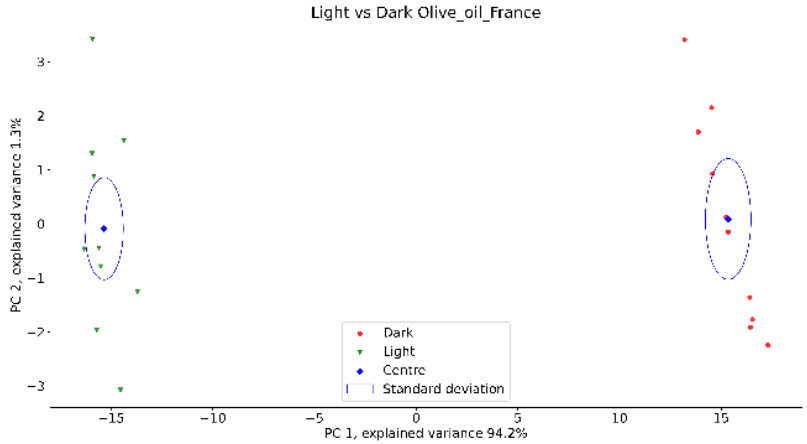

Average absorbance spectra of light and dark Mustard_delhi
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

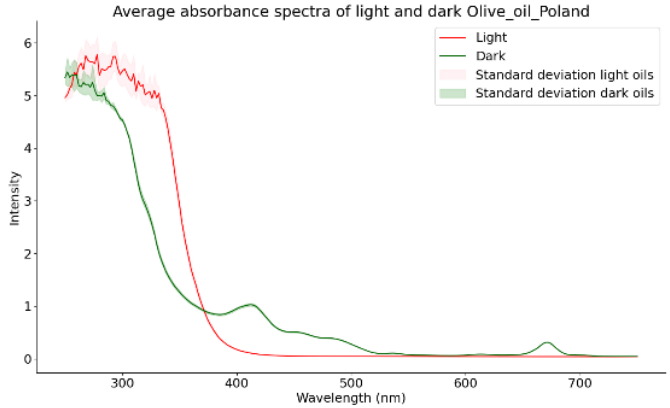

Light vs Dark Mustard_delhi
Dark
Light
Centre
Standard deviation
PC 2, explained variance 25.0%
PC 1, explained variance 67.8%

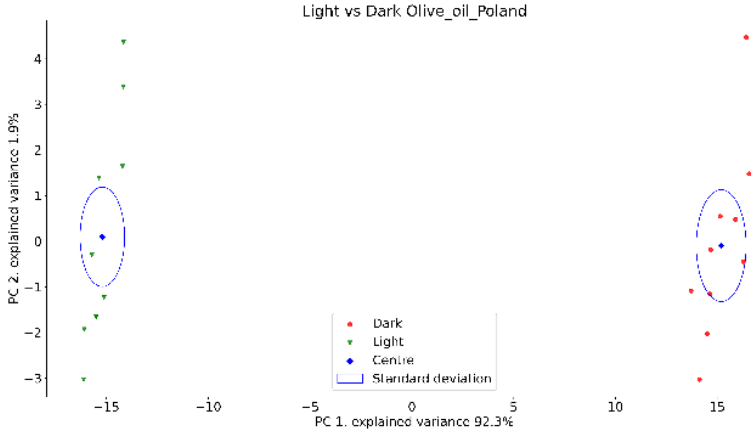

Average absorbance spectra of light and dark Oelh
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

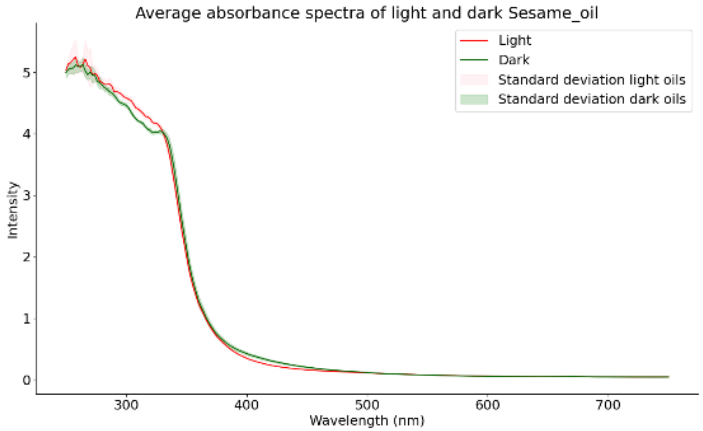

Light vs Dark Oelh
Dark
Light
Centre
Standard deviation
PC 2, explained variance 16.0%
PC 1, explained variance 65.4%

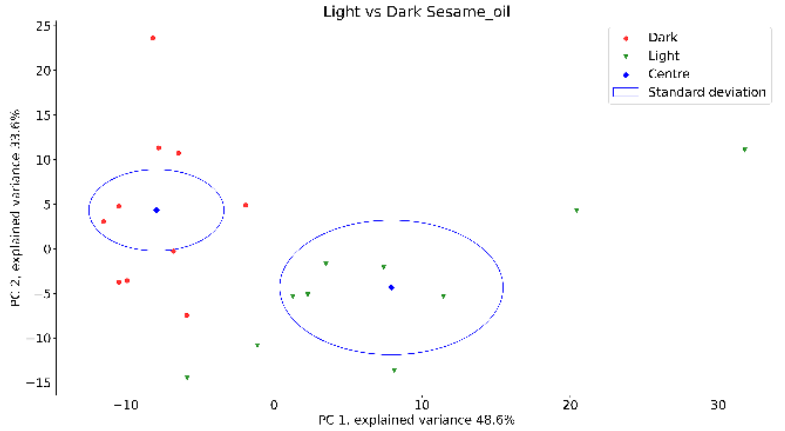

Average absorbance spectra of light and dark Olive_oil_France
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

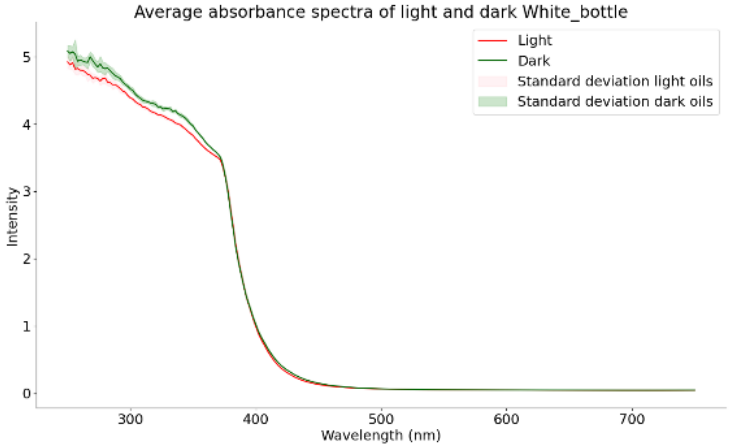

Light vs Dark Olive_oil_France
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.3%
PC 1, explained variance 94.2%

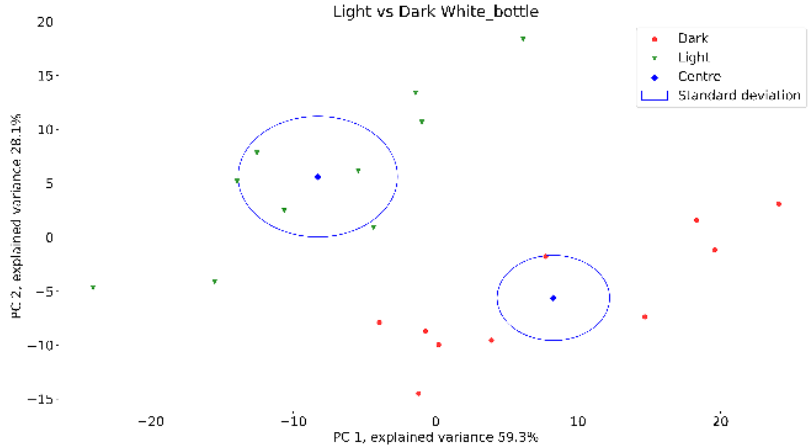

Average absorbance spectra of light and dark Olive_oil_Poland
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)


Light vs Dark Olive_oil_Poland
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.9%
PC 1, explained variance 92.3%


Average absorbance spectra of light and dark Sesame_oil
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

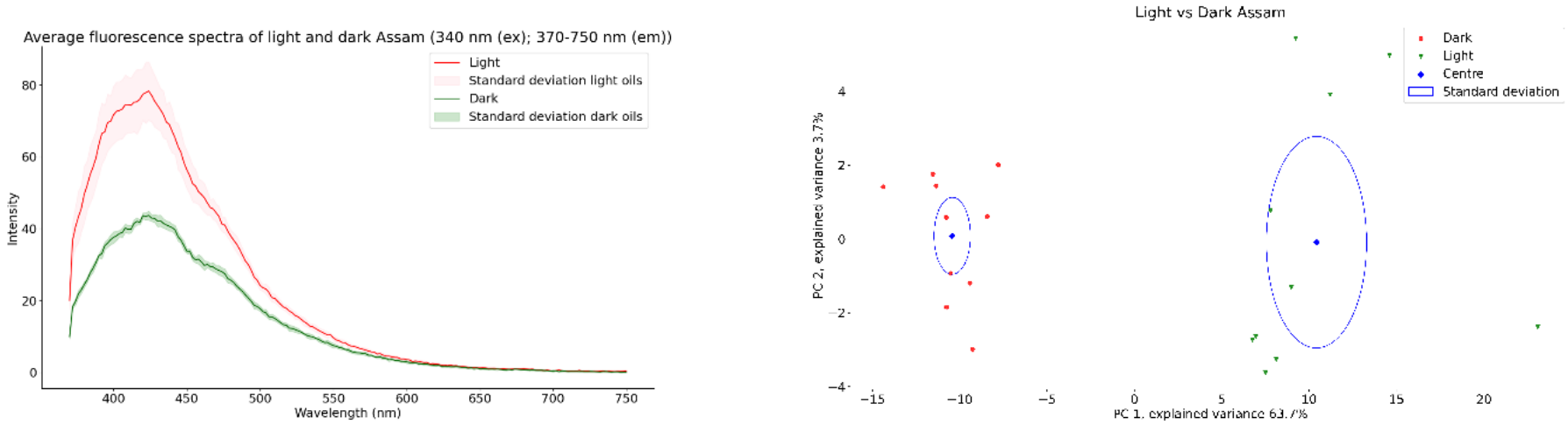

Light vs Dark Sesame_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 33.6%
PC 1, explained variance 48.6%

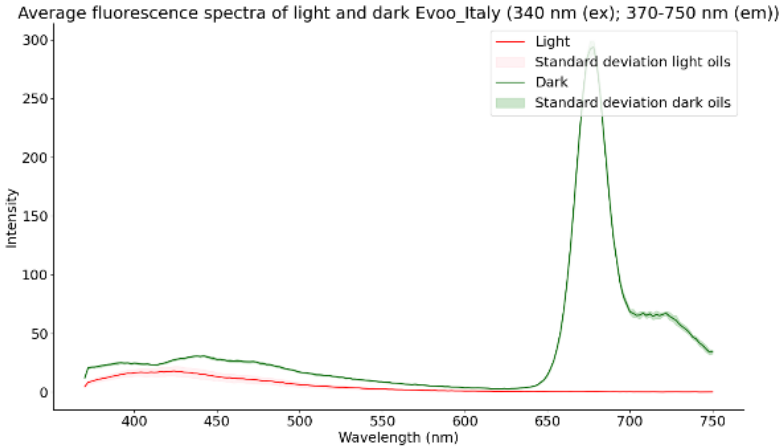

Average absorbance spectra of light and dark White_bottle
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

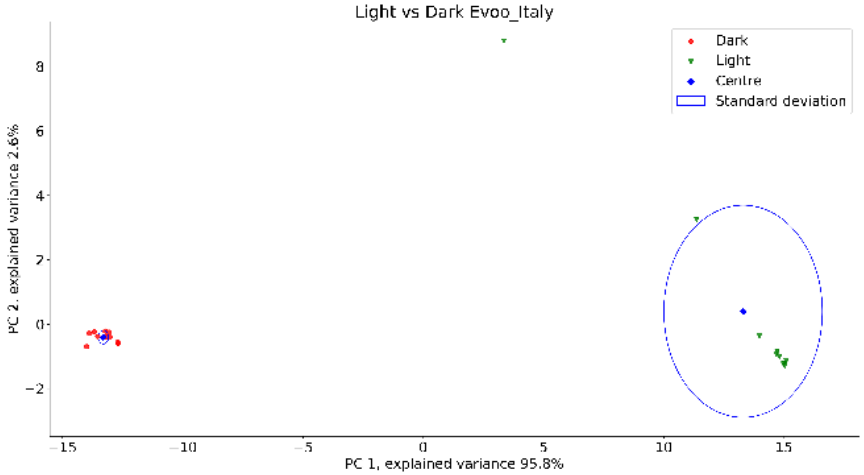

Light vs Dark White_bottle
Dark
Light
Centre
Standard deviation
PC 2, explained variance 28.1%
PC 1, explained variance 59.3%

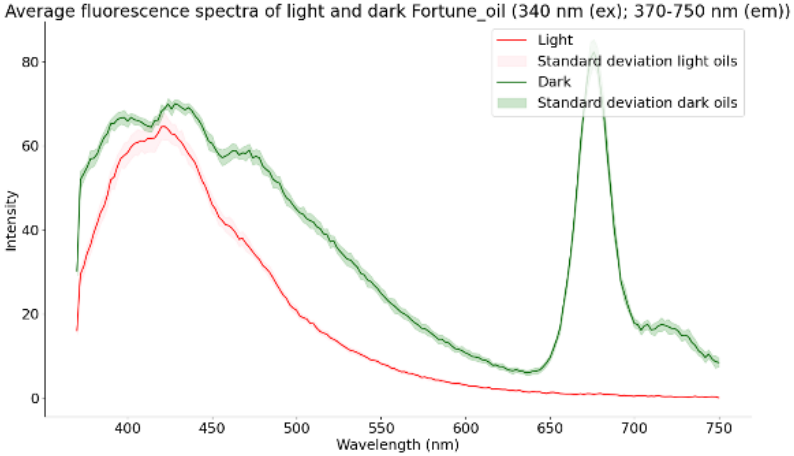
APPENDIX B

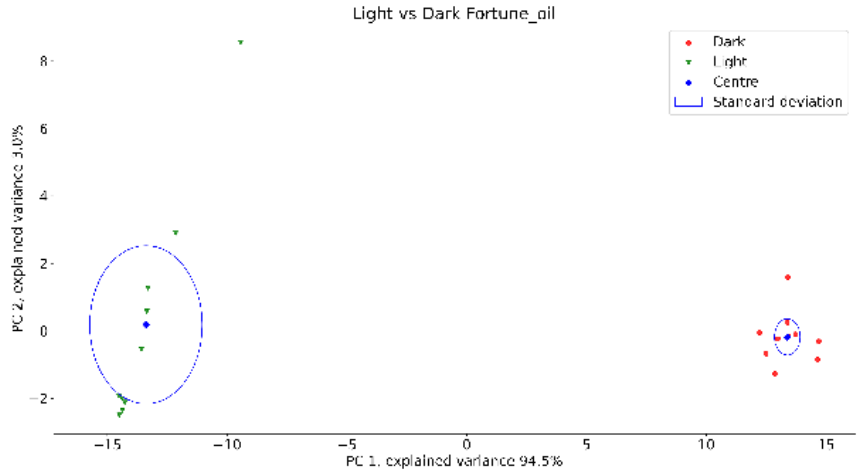
Figure B.1 - The results of analysis of Fluorescence (340 nm (ex), 370-750 nm (em)) oils data analysis and PCA visualization.

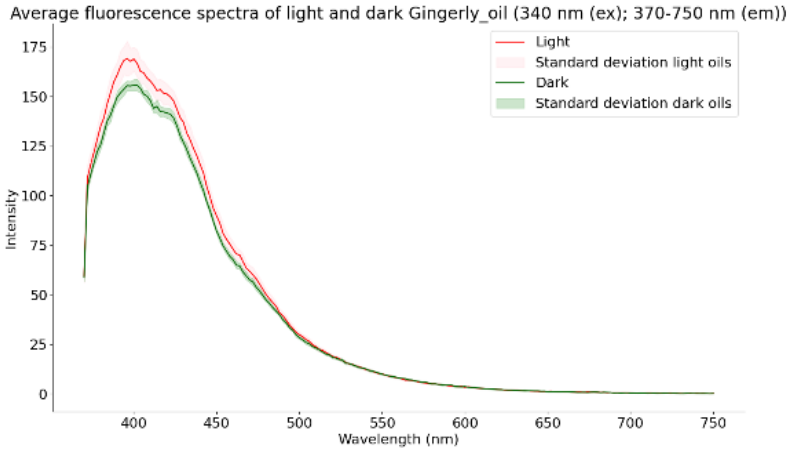


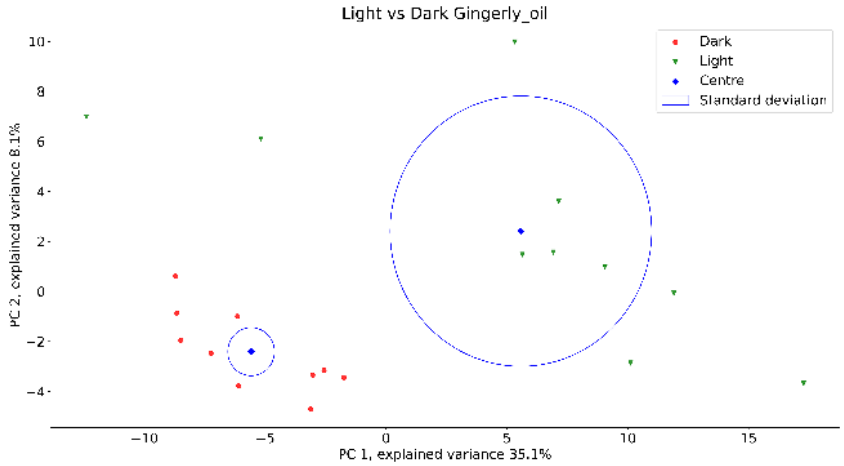

Average fluorescence spectra of light and dark Evoo_Italy (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

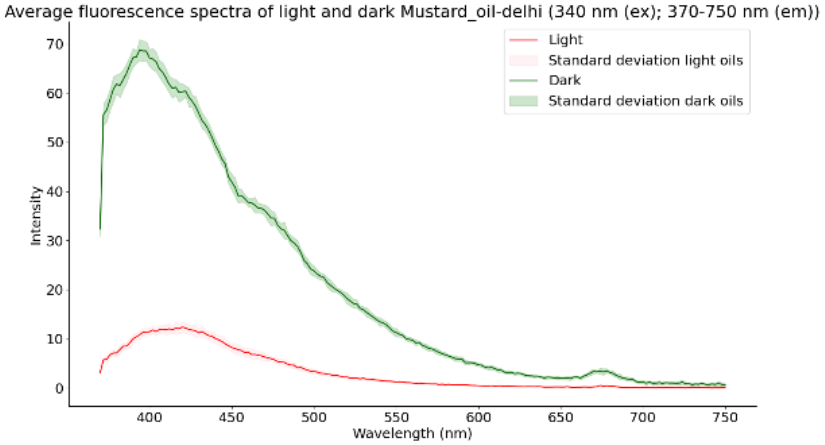

Light vs Dark Evoo_Italy
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.6%
PC 1, explained variance 95.8%

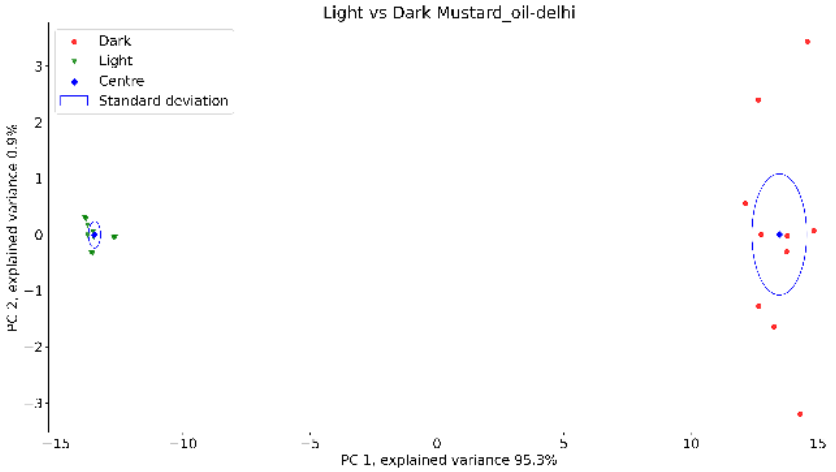

Average fluorescence spectra of light and dark Fortune_oil (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

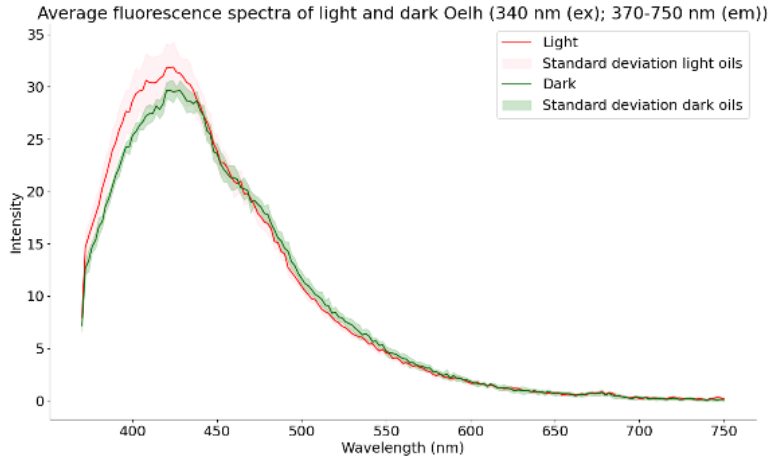

Light vs Dark Fortune_oil
Dark
Light
Centre
Standard deviation
PC 1, explained variance 94.5%

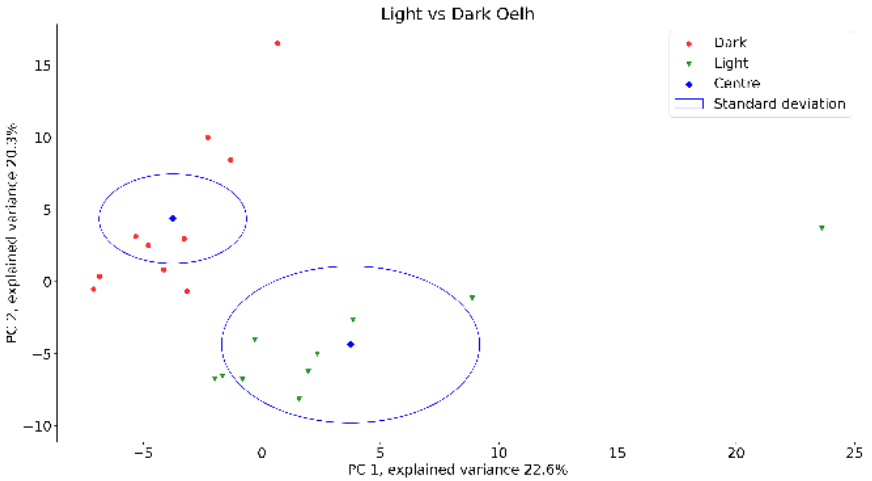

Average fluorescence spectra of light and dark Gingerly_oil (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

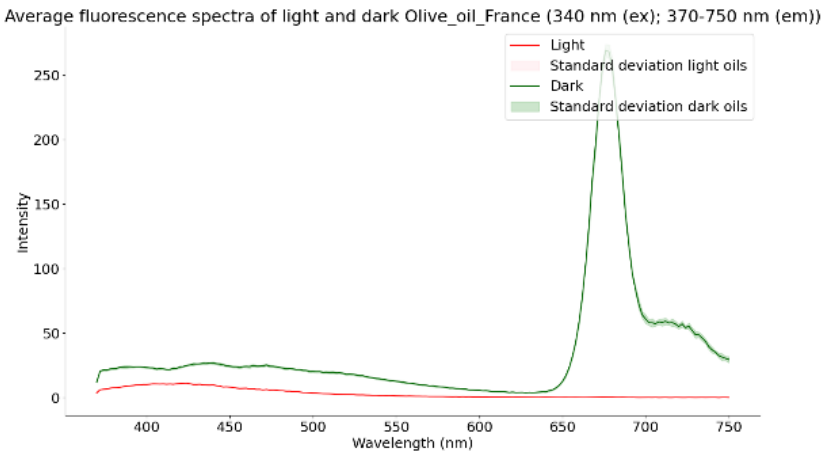

Light vs Dark Gingerly_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 8.1%
PC 1, explained variance 35.1%

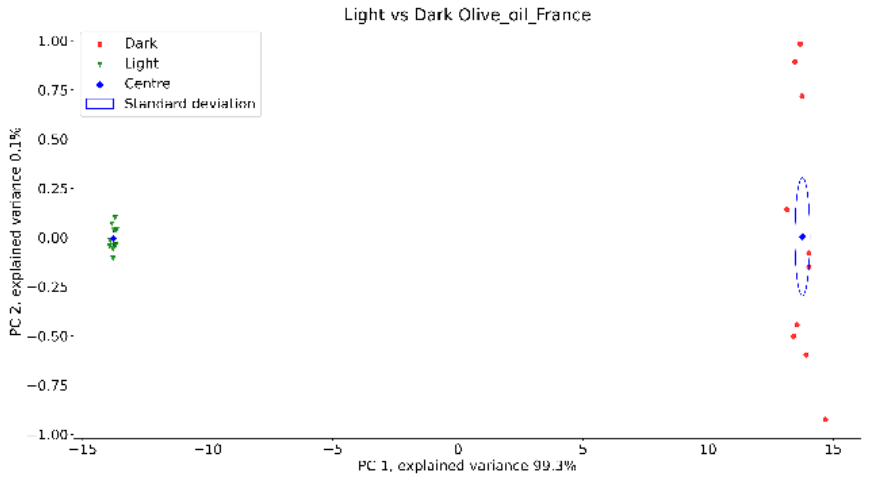

Average fluorescence spectra of light and dark Mustard_oil-delhi (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

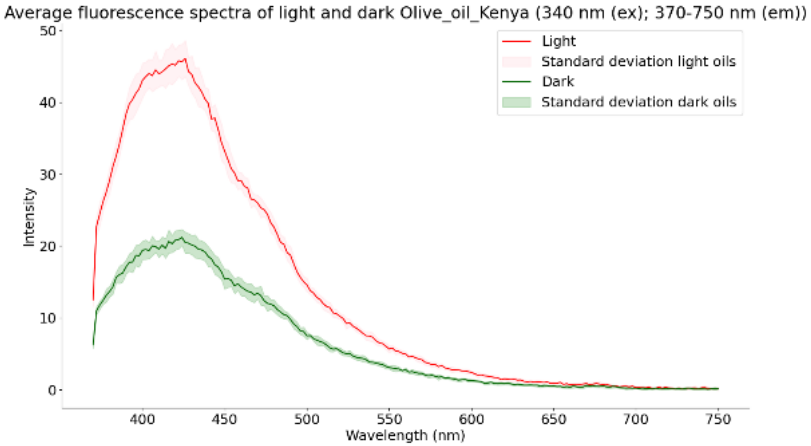

Light vs Dark Mustard_oil-delhi
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.9%
PC 1, explained variance 95.3%

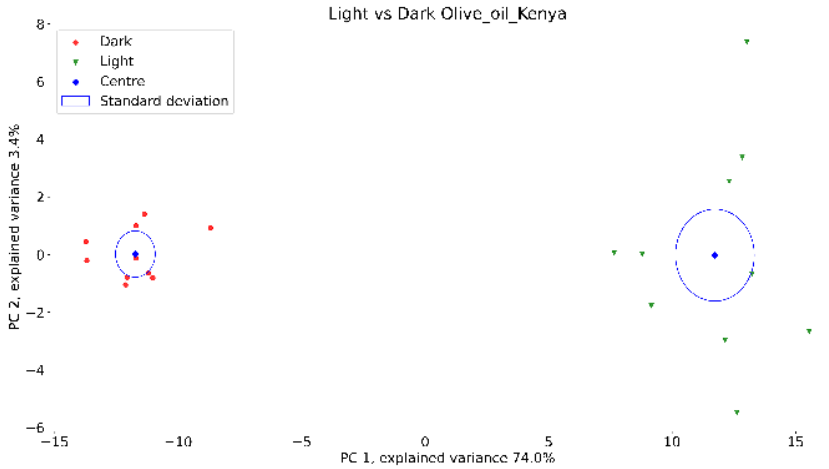

Average fluorescence spectra of light and dark Oelh (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

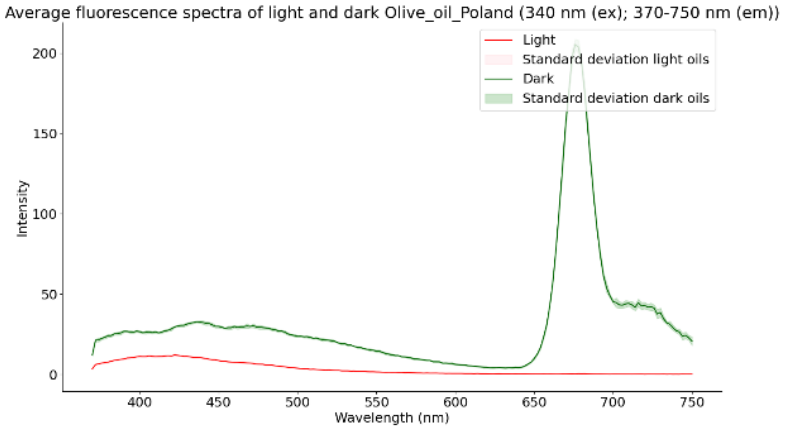

Light vs Dark Oelh
Dark
Light
Centre
Standard deviation
PC 2, explained variance 20.3%
PC 1, explained variance 22.6%

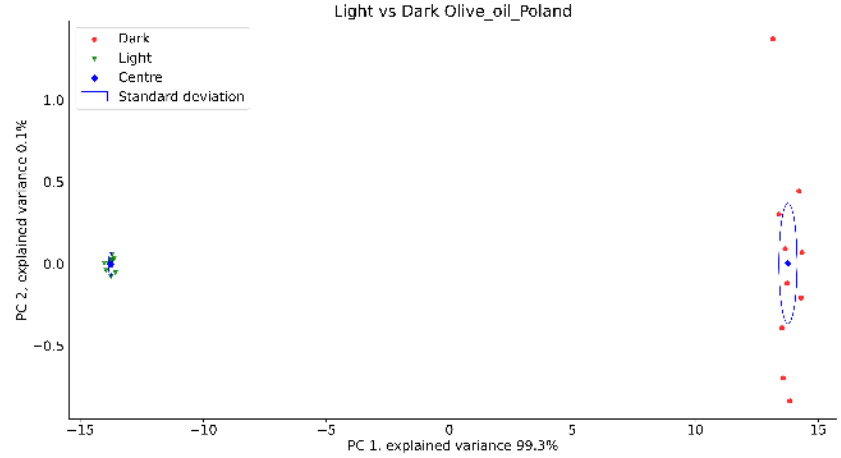

Average fluorescence spectra of light and dark Olive_oil_France (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

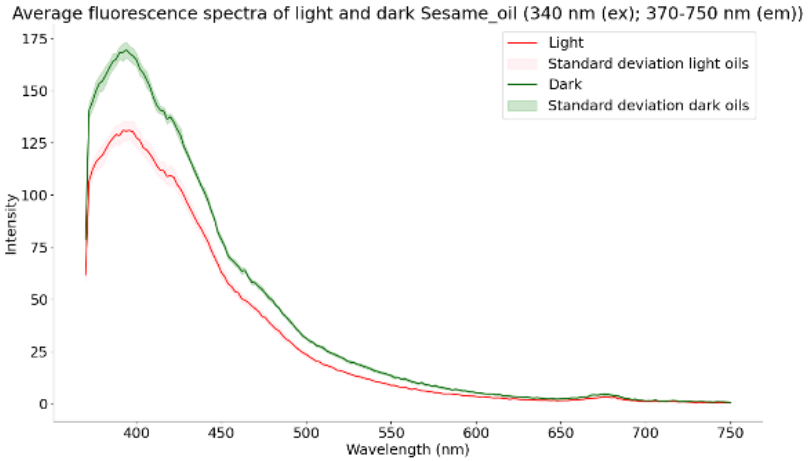

Light vs Dark Olive_oil_France
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.1%
PC 1, explained variance 99.3%

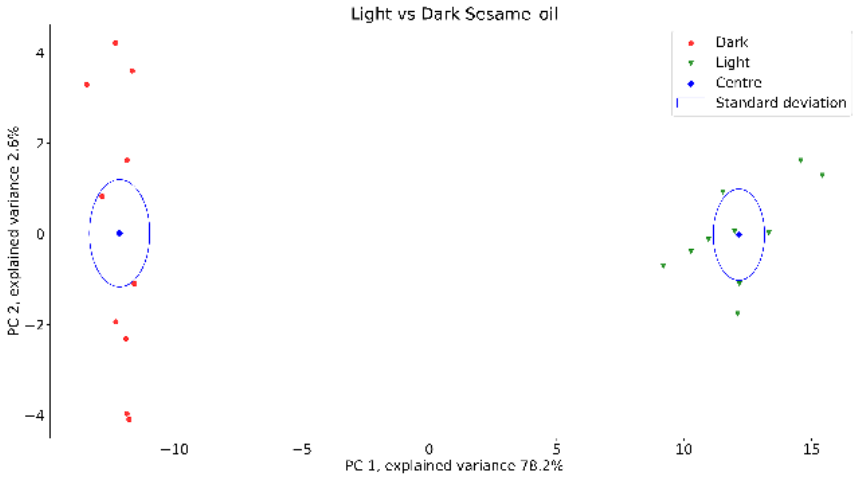

Average fluorescence spectra of light and dark Olive_oil_Kenya (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

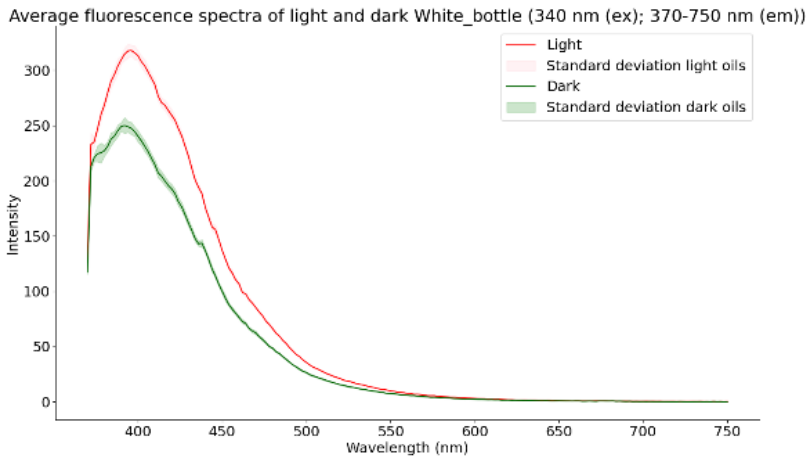

Light vs Dark Olive_oil_Kenya
Dark
Light
Centre
Standard deviation
PC 2, explained variance 3.4%
PC 1, explained variance 74.0%

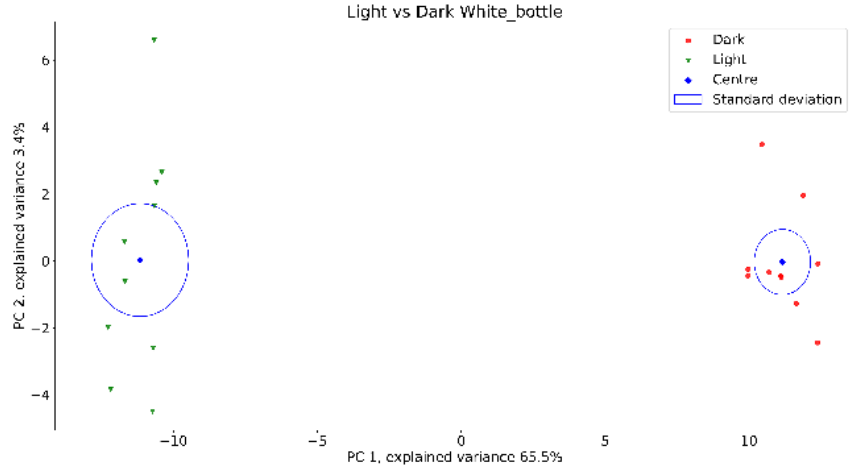

Average fluorescence spectra of light and dark Olive_oil_Poland (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)


Light vs Dark Olive_oil_Poland
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.1%
PC 1, explained variance 99.3%


Average fluorescence spectra of light and dark Sesame_oil (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

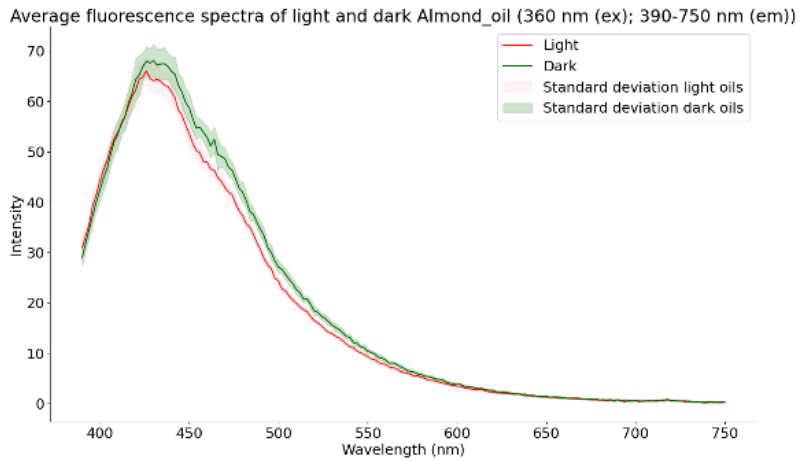

Light vs Dark Sesame oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.6%
PC 1, explained variance 78.2%

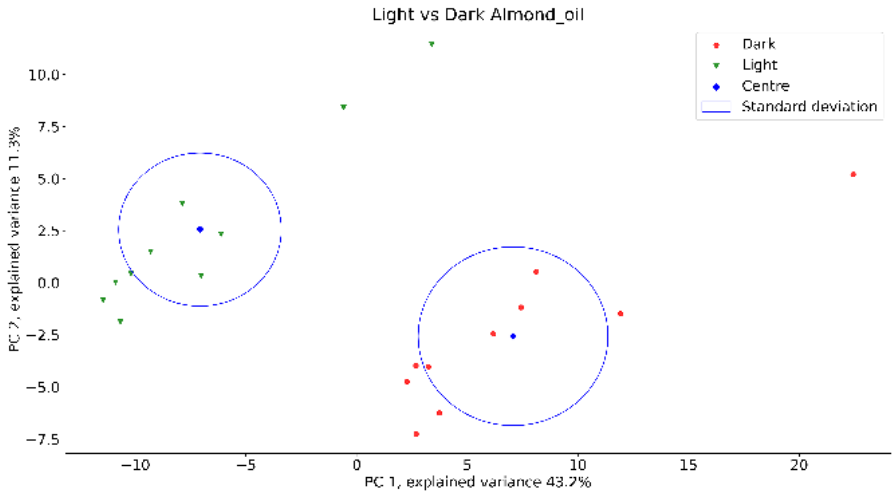

Average fluorescence spectra of light and dark White_bottle (340 nm (ex); 370-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

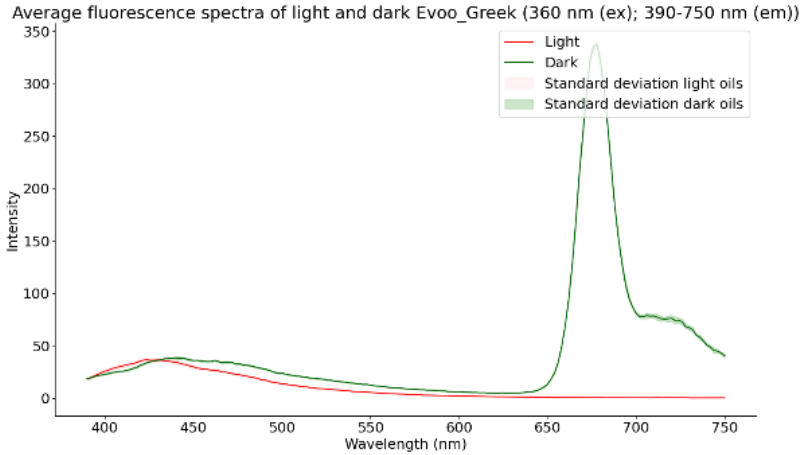

Light vs Dark White_bottle
Dark
Light
Centre
Standard deviation
PC 2, explained variance 3.4%
PC 1, explained variance 65.5%

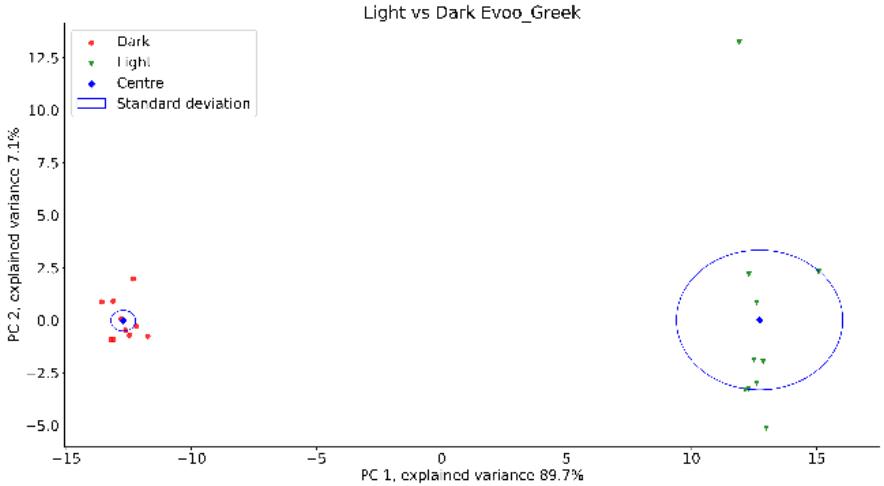
APPENDIX C.

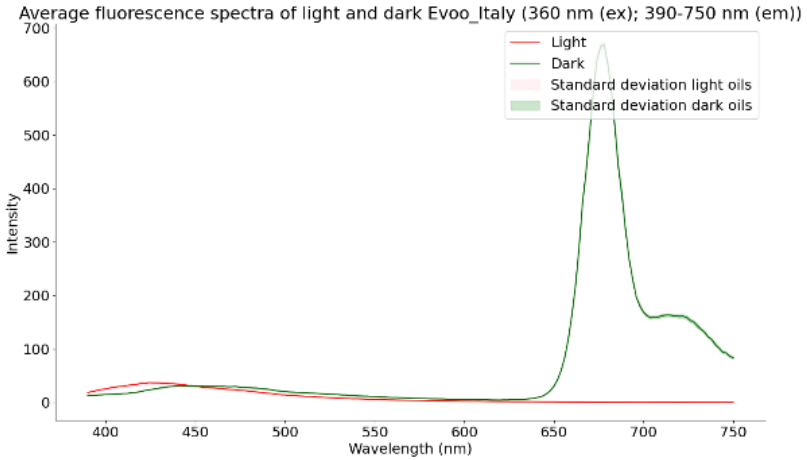
Figure C.1 - The results of analysis of Fluorescence (360 nm (ex), 390-750 nm (em)) oils data analysis and PCA visualization.

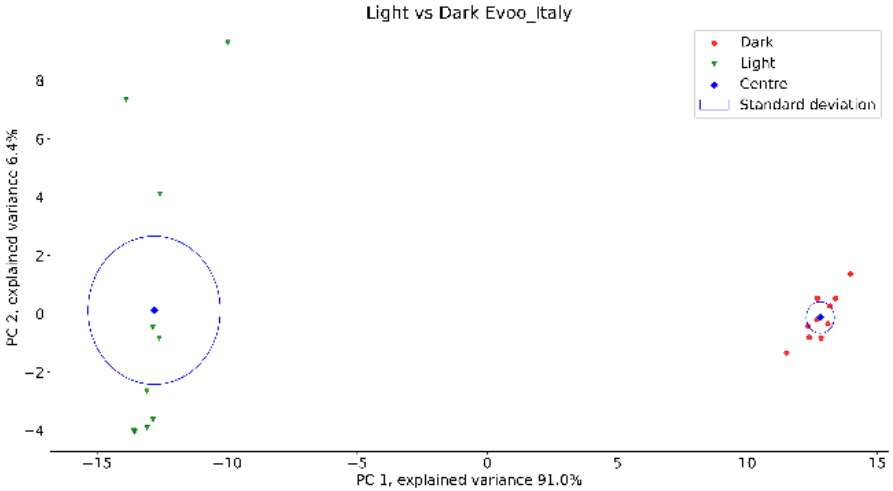


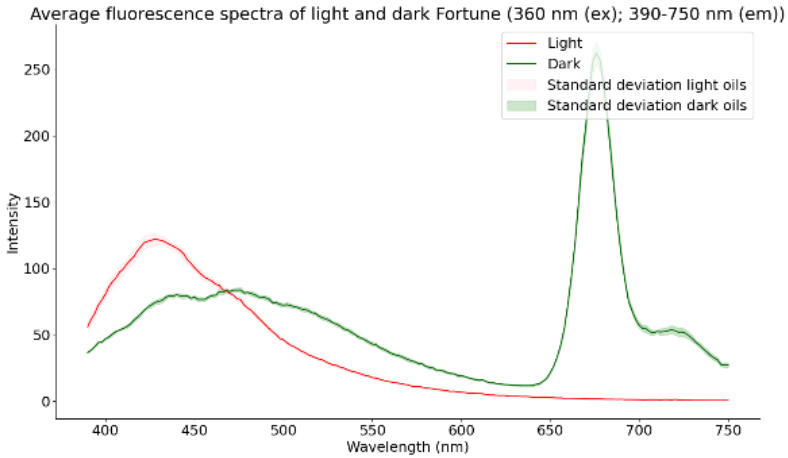


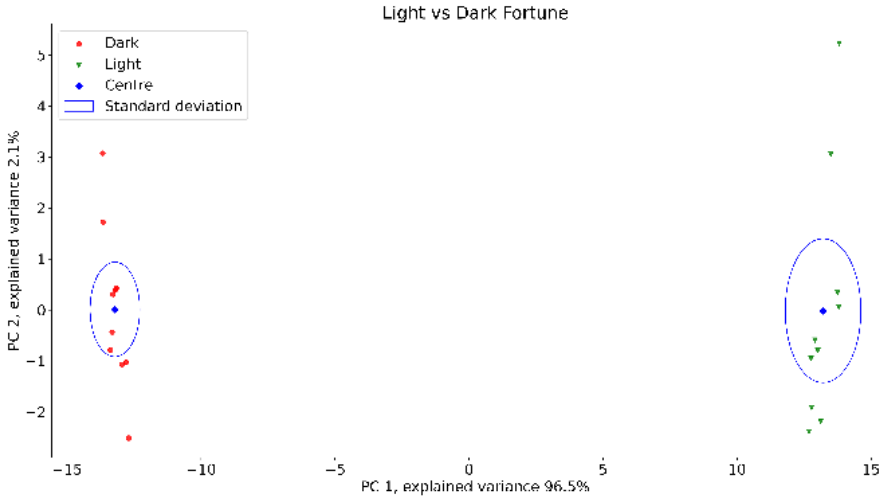

Average fluorescence spectra of light and dark Evoo_Greek (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

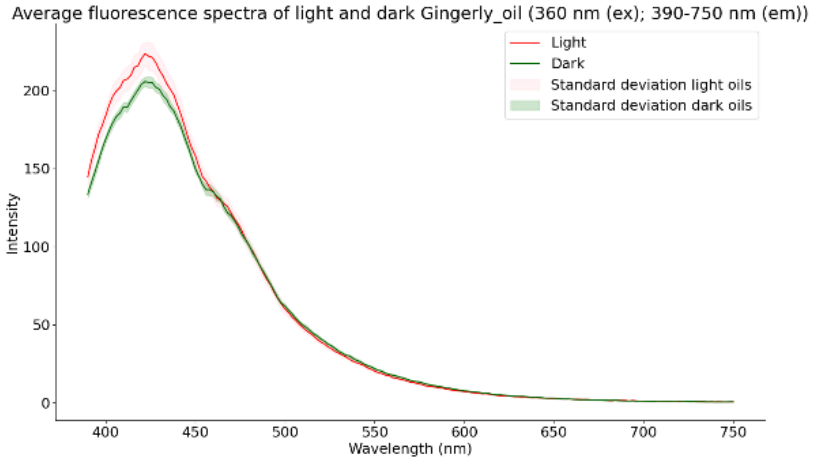

Light vs Dark Evoo_Greek
Dark
Light
Centre
Standard deviation
PC 2, explained variance 7.1%
PC 1, explained variance 89.7%

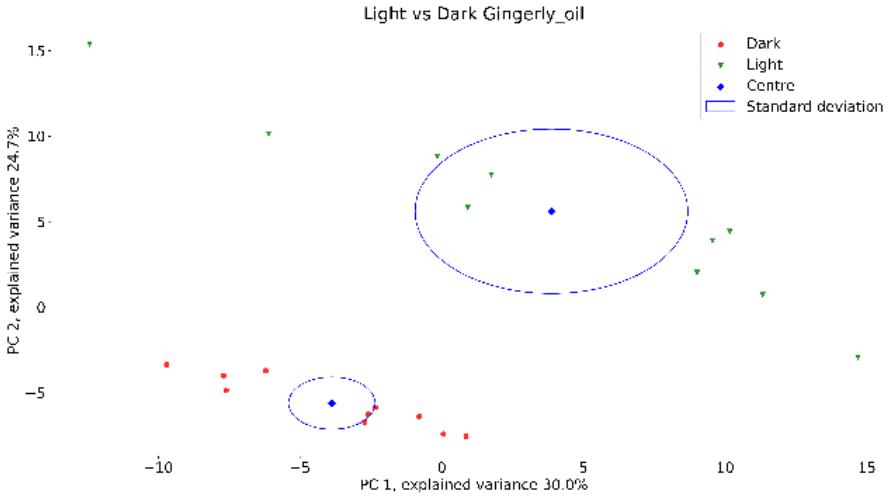

Average fluorescence spectra of light and dark Evoo_Italy (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

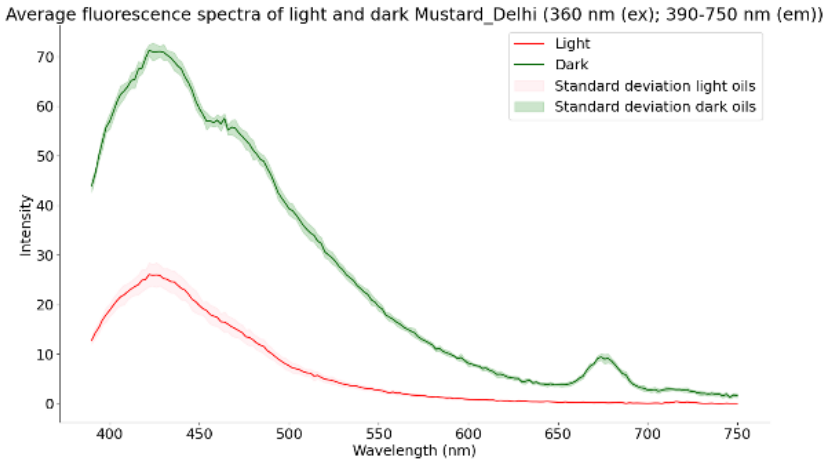

Light vs Dark Evoo_Italy
Dark
Light
Centre
Standard deviation
PC 2, explained variance 6.4%
PC 1, explained variance 91.0%

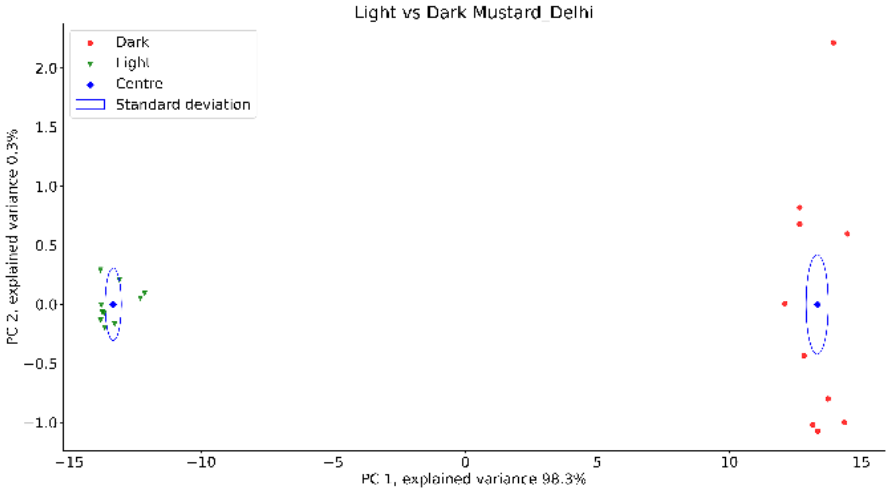

Average fluorescence spectra of light and dark Fortune (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

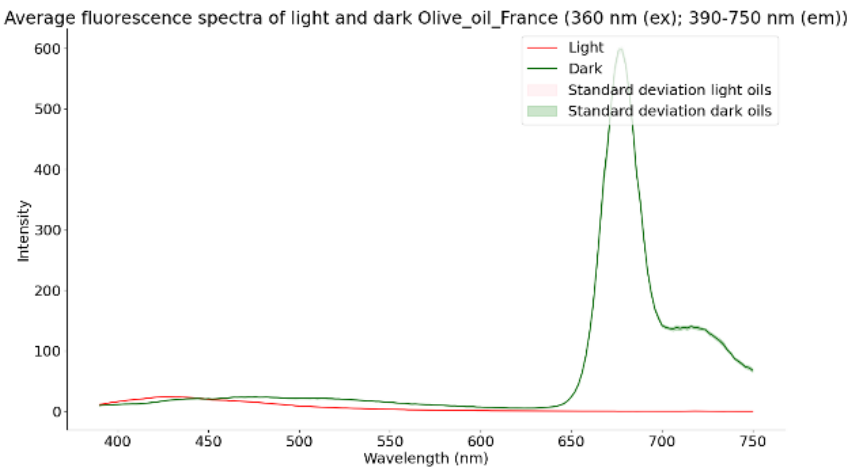

Light vs Dark Fortune
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.1%
PC 1, explained variance 96.5%

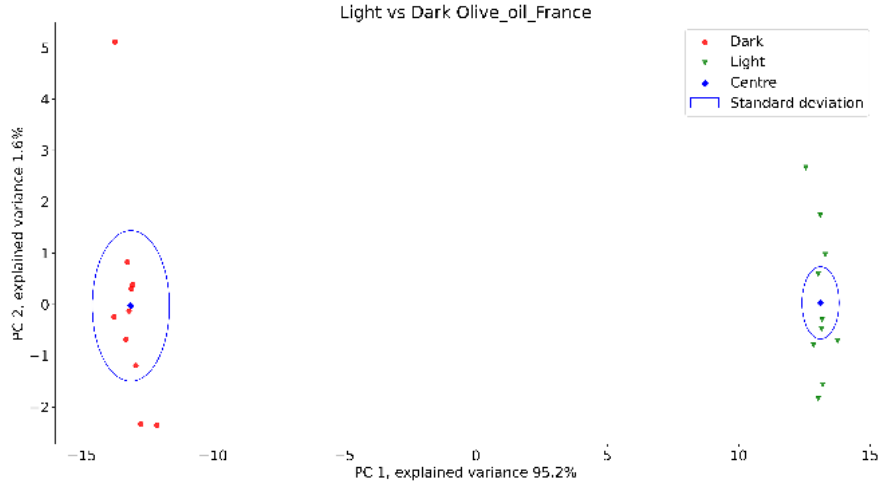

Average fluorescence spectra of light and dark Gingerly_oil (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

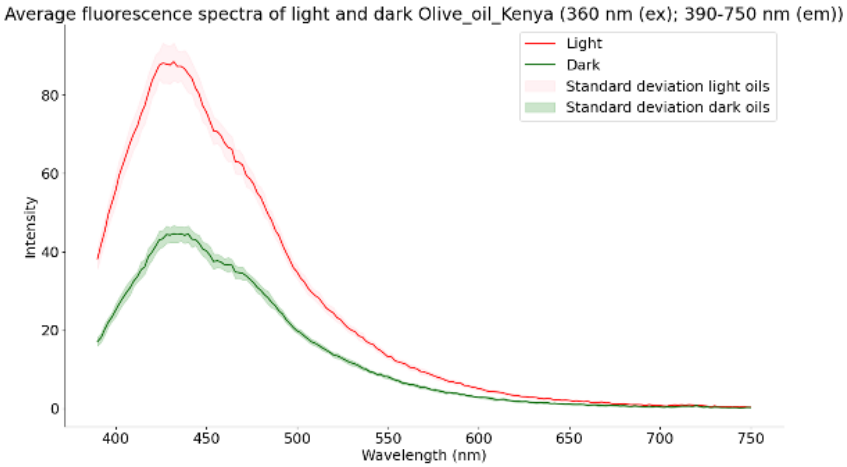

Light vs Dark Gingerly_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 24.7%
PC 1, explained variance 30.0%

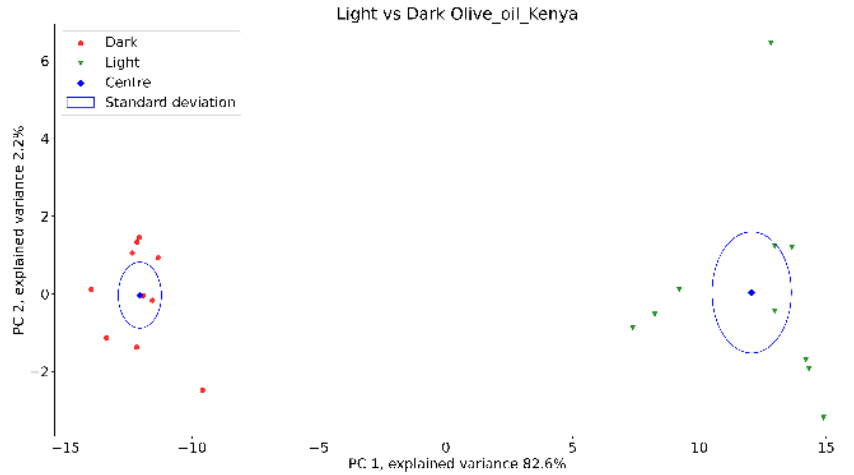

Average fluorescence spectra of light and dark Mustard_Delhi (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

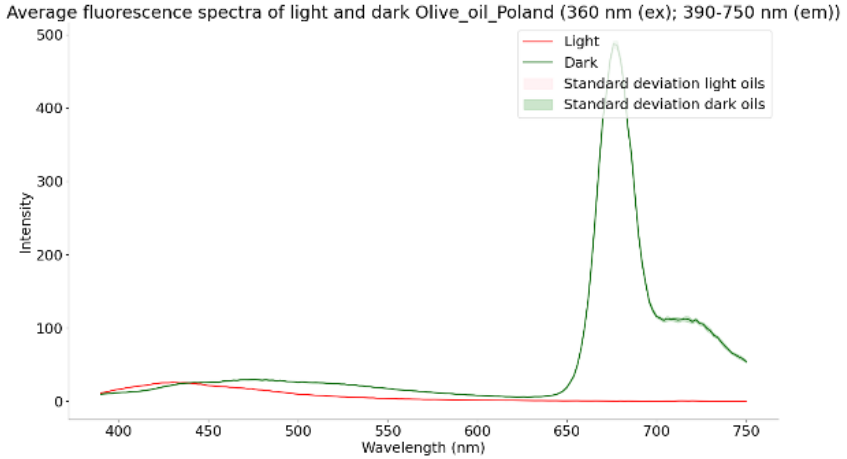

Light vs Dark Mustard_Delhi
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.3%
PC 1, explained variance 98.3%

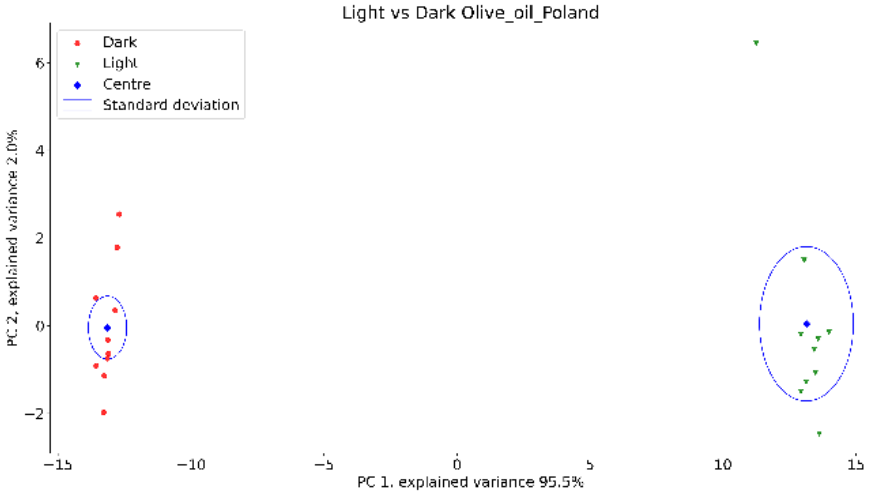

Average fluorescence spectra of light and dark Olive_oil_France (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

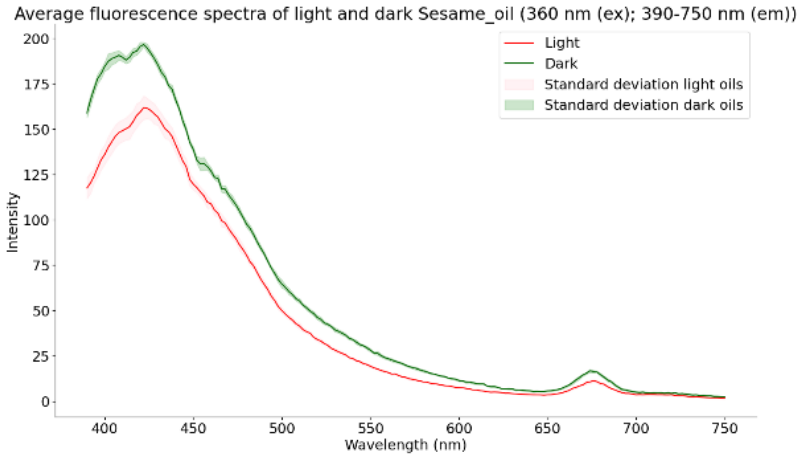

Light vs Dark Olive_oil_France
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.6%
PC 1, explained variance 95.2%

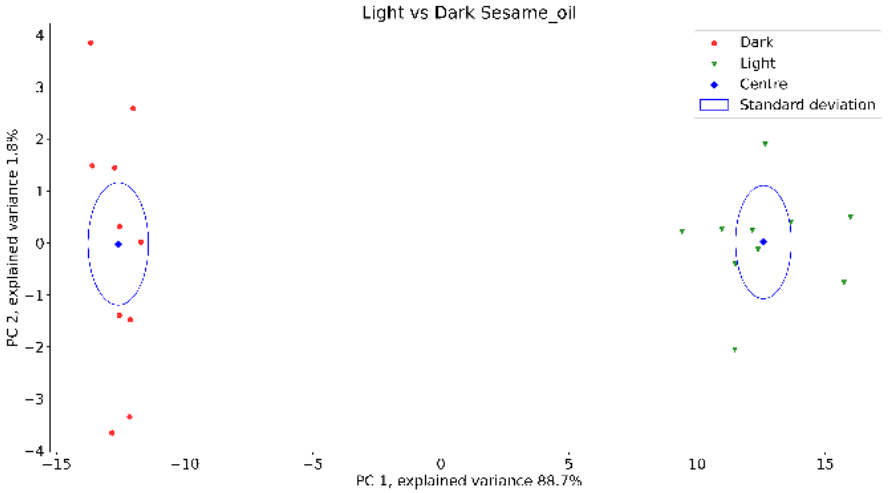

Average fluorescence spectra of light and dark Olive_oil_Kenya (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

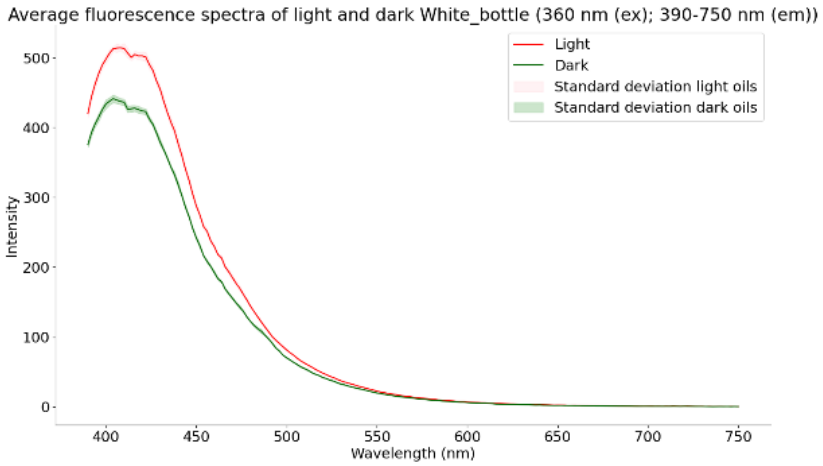

Light vs Dark Olive_oil_Kenya
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.2%
PC 1, explained variance 82.6%

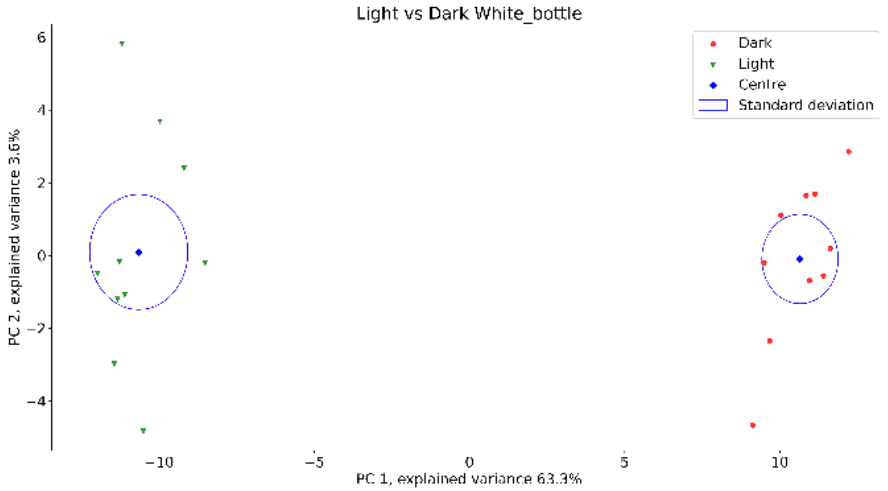

Average fluorescence spectra of light and dark Olive_oil_Poland (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)


Light vs Dark Olive_oil_Poland
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.0%
PC 1, explained variance 95.5%


Average fluorescence spectra of light and dark Sesame_oil (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

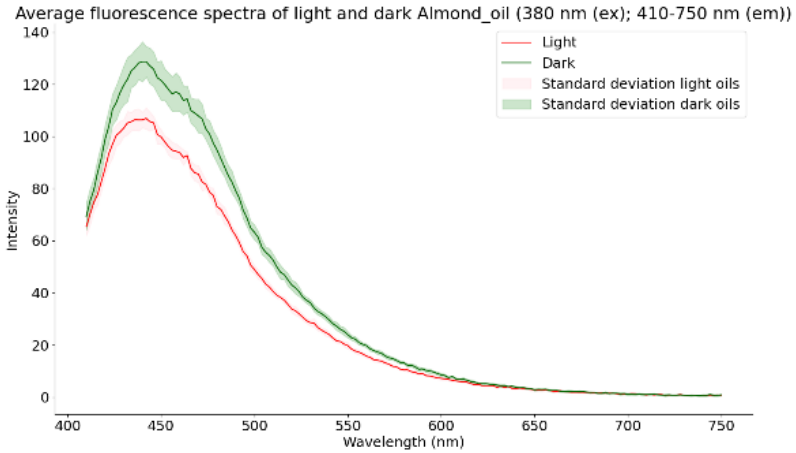

Light vs Dark Sesame_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.8%
PC 1, explained variance 88.7%

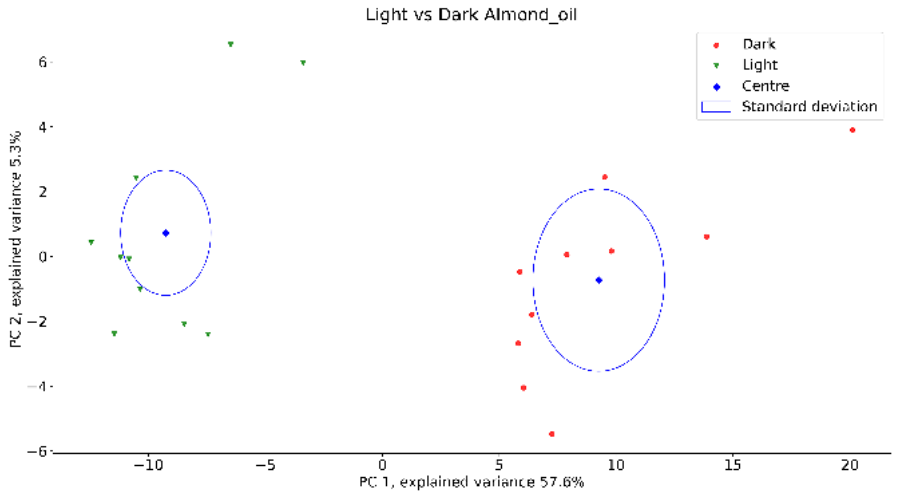

Average fluorescence spectra of light and dark White_bottle (360 nm (ex); 390-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

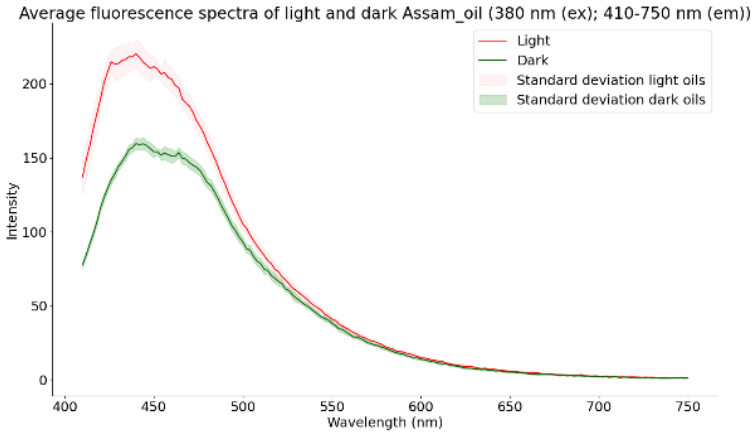

Light vs Dark White_bottle
Dark
Light
Centre
Standard deviation
PC 2, explained variance 3.6%
PC 1, explained variance 63.3%

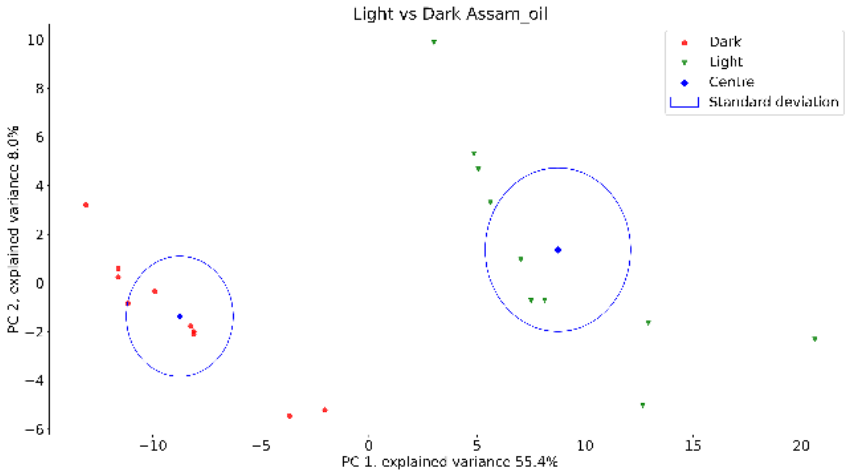
APPENDIX D

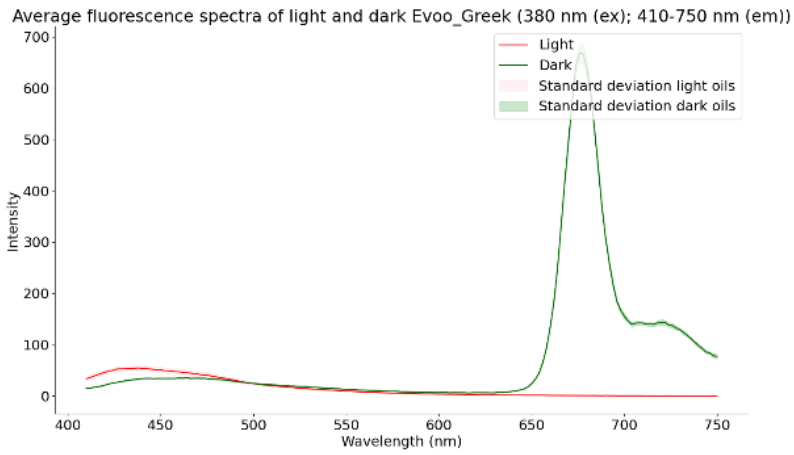
Figure D.1 - The results of analysis of Fluorescence (380 nm (ex), 410-750 nm (em)) oils data analysis and PCA visualization.

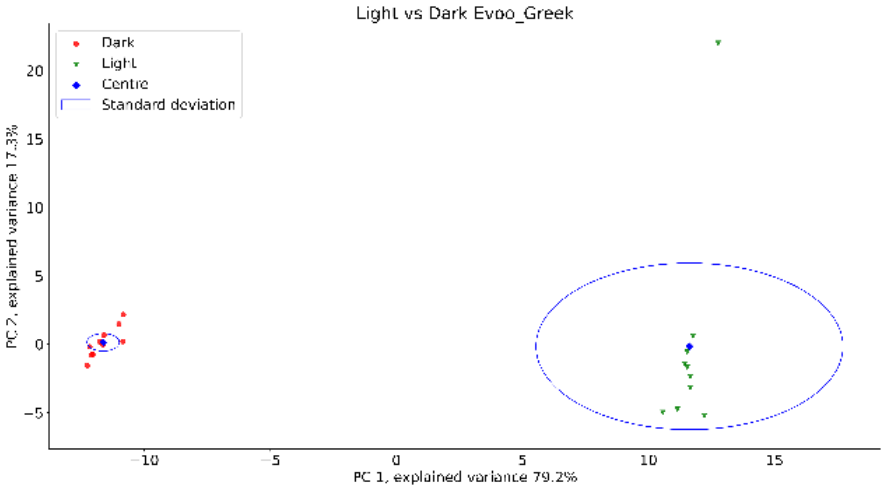


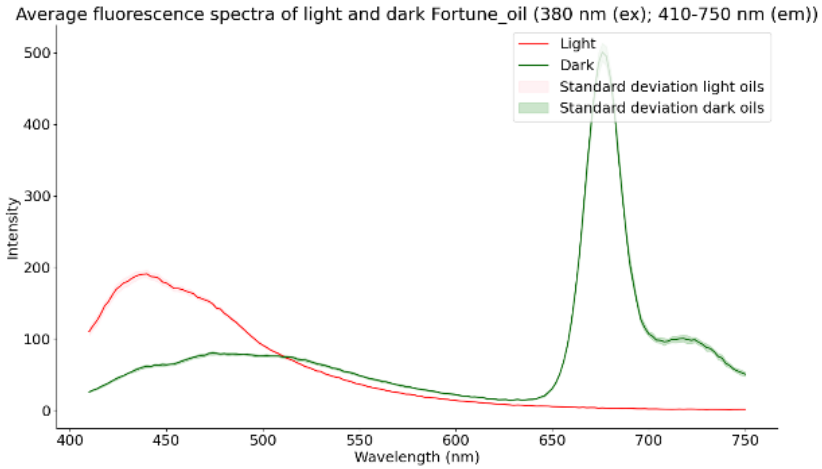


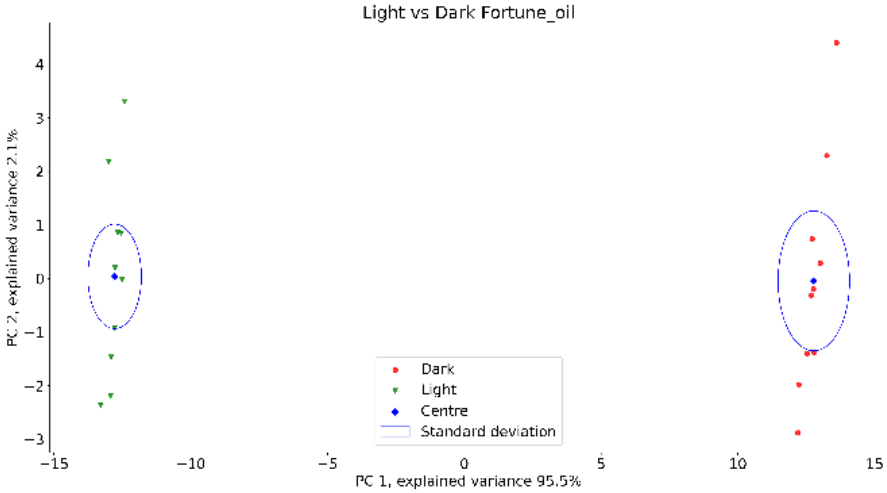

Average fluorescence spectra of light and dark Assam_oil (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

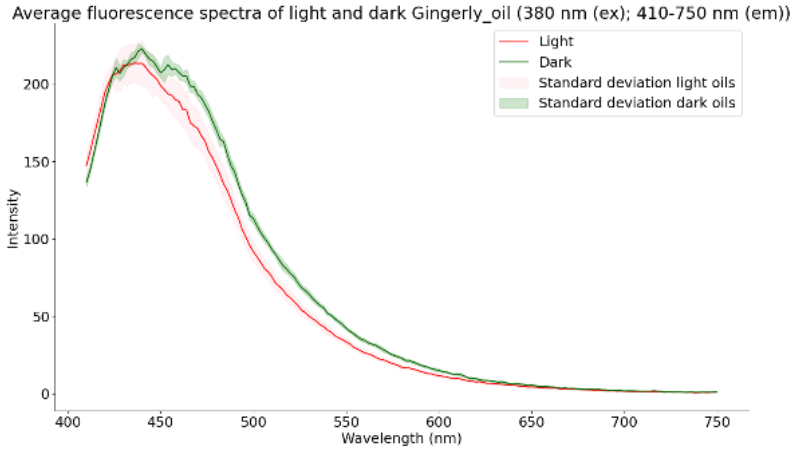

Light vs Dark Assam_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 8.0%
PC 1, explained variance 55.4%

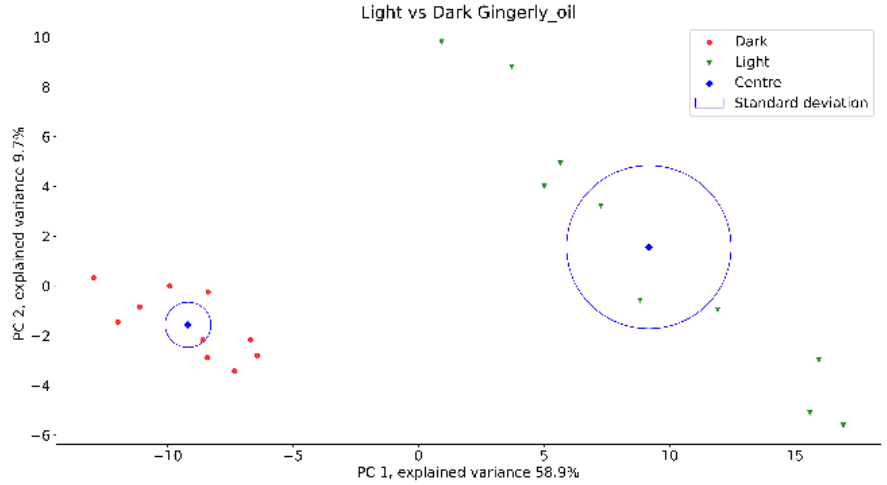

Average fluorescence spectra of light and dark Evoo_Greek (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

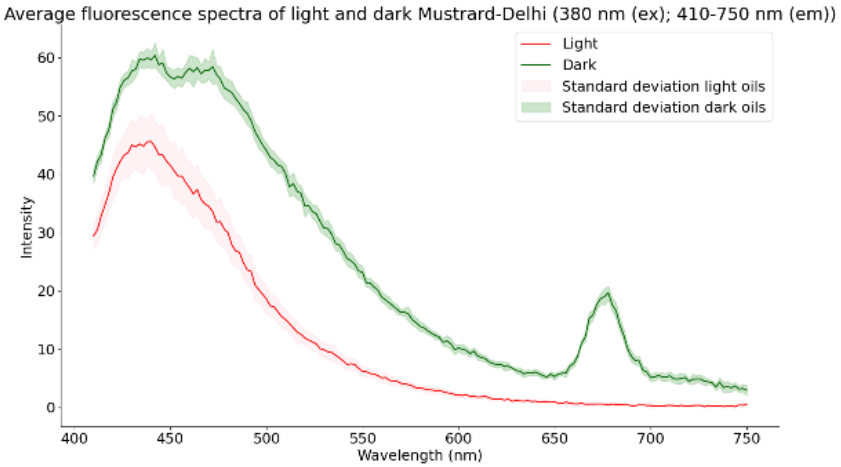

Light vs Dark Evoo_Greek
Dark
Light
Centre
Standard deviation
PC 2, explained variance 17.3%
PC 1, explained variance 79.2%

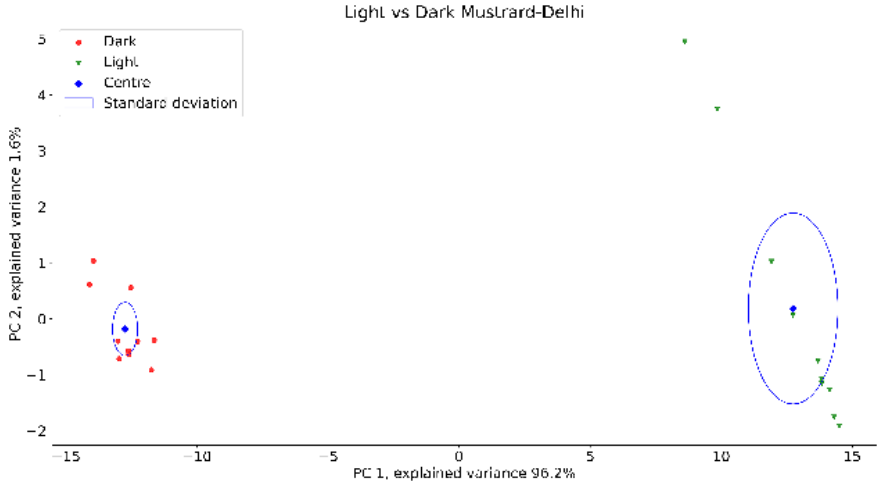

Average fluorescence spectra of light and dark Fortune_oil (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

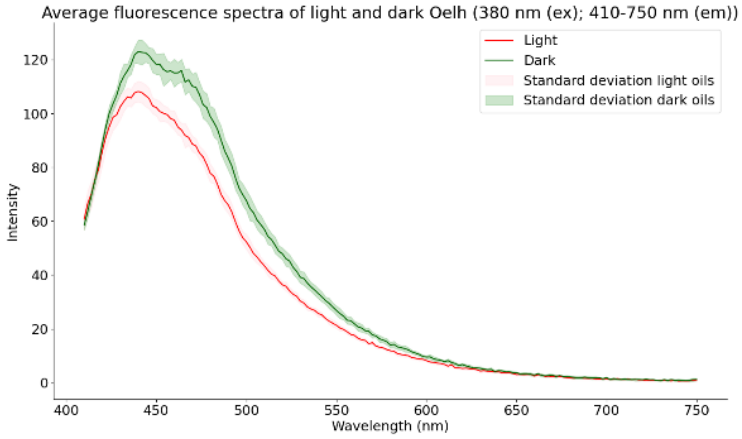

Light vs Dark Fortune_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.1%
PC 1, explained variance 95.5%

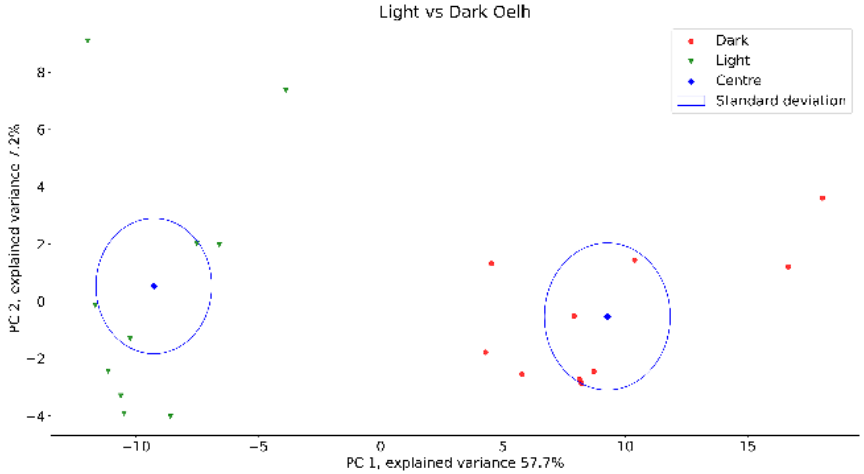

Average fluorescence spectra of light and dark Gingerly_oil (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

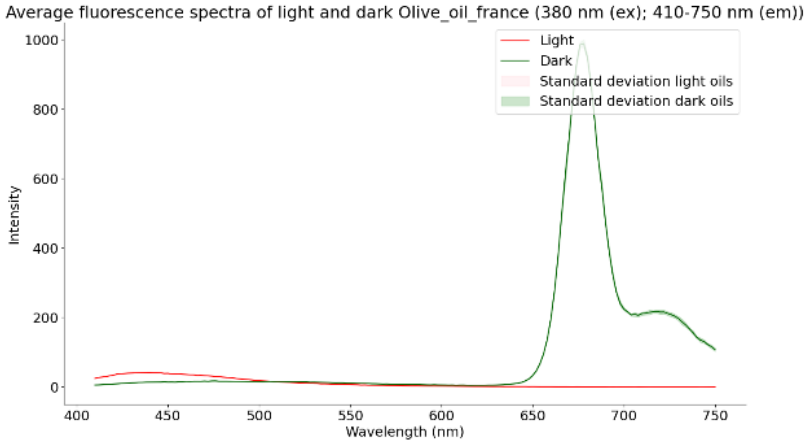

Light vs Dark Gingerly_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 9.7%
PC 1, explained variance 58.9%

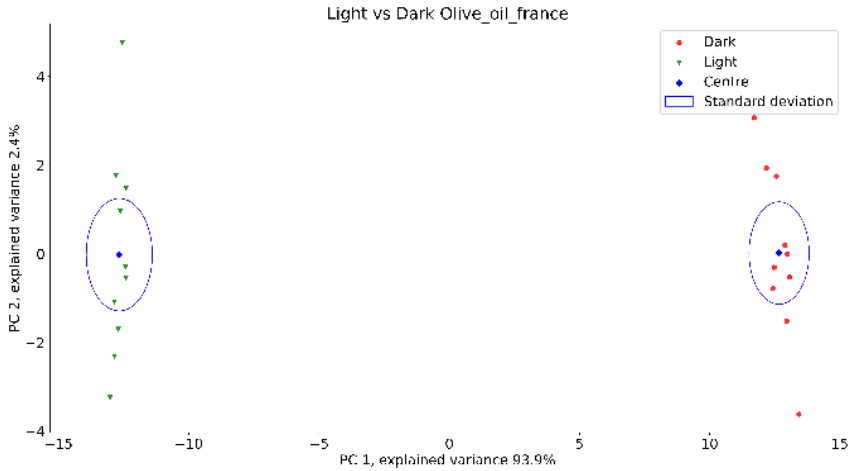

Average fluorescence spectra of light and dark Mustrard-Delhi (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

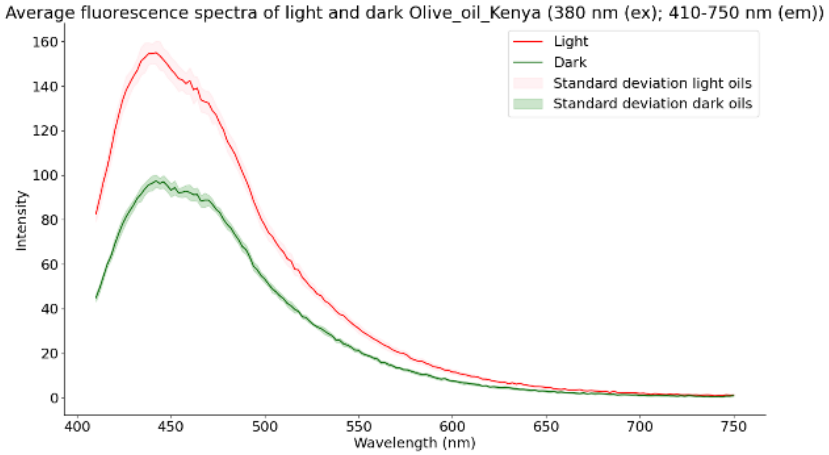

Light vs Dark Mustrard-Delhi
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.6%
PC 1, explained variance 96.2%

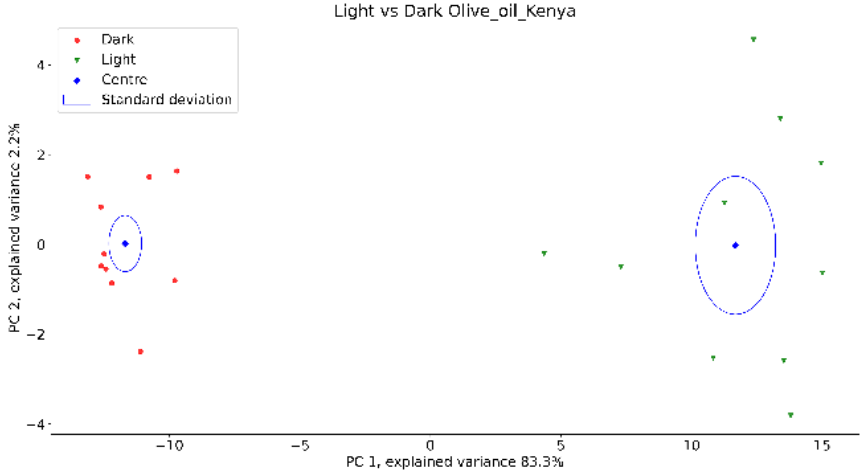

Average fluorescence spectra of light and dark Oelh (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

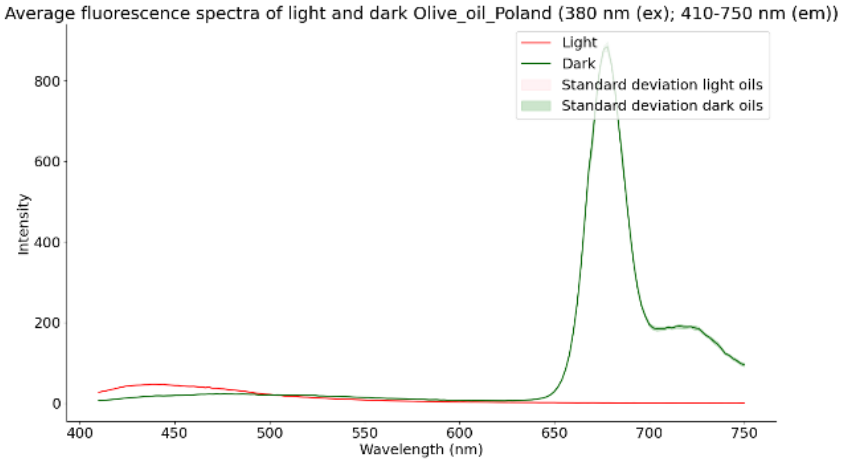

Light vs Dark Oelh
Dark
Light
Centre
Standard deviation
PC 2, explained variance 7.2%
PC 1, explained variance 57.7%

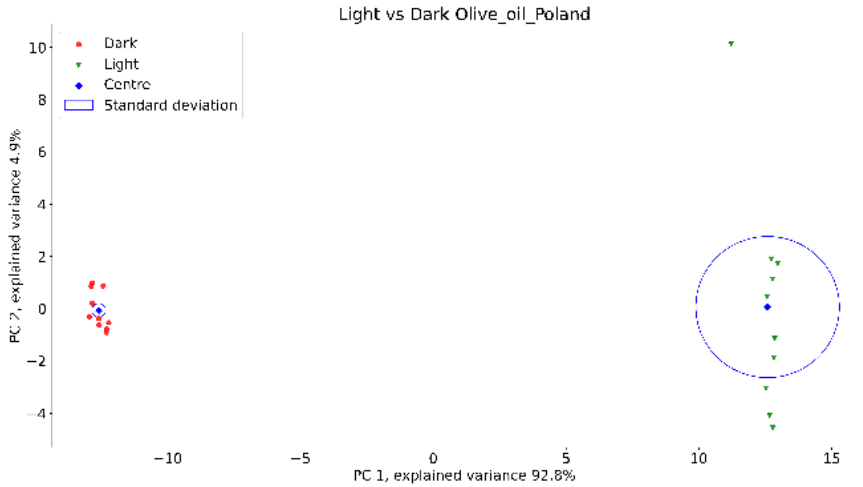

Average fluorescence spectra of light and dark Olive_oil_france (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

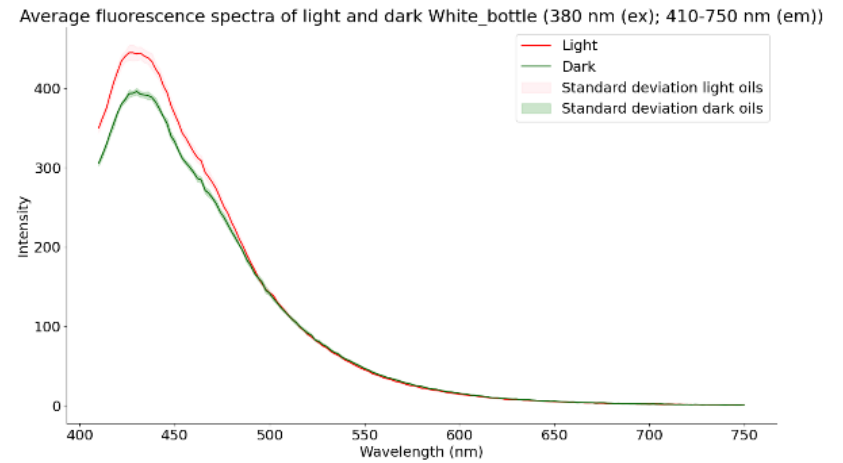

Light vs Dark Olive_oil_france
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.4%
PC 1, explained variance 93.9%

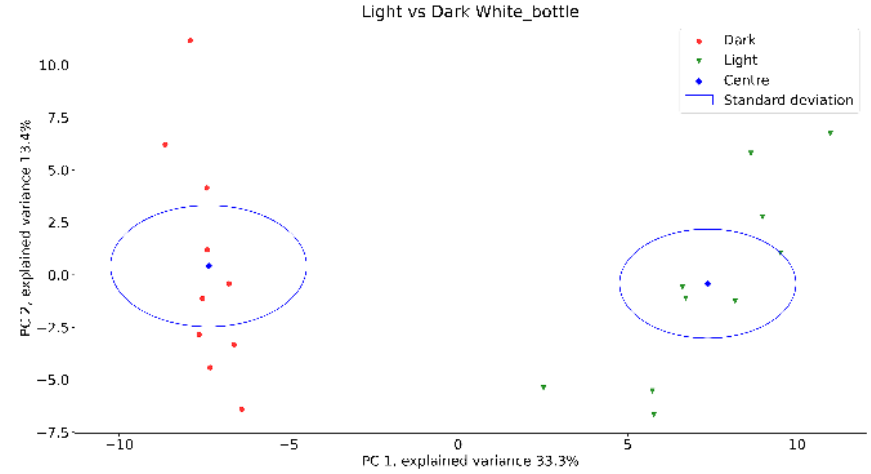

Average fluorescence spectra of light and dark Olive_oil_Kenya (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)


Light vs Dark Olive_oil_Kenya
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.2%
PC 1, explained variance 83.3%


Average fluorescence spectra of light and dark Olive_oil_Poland (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

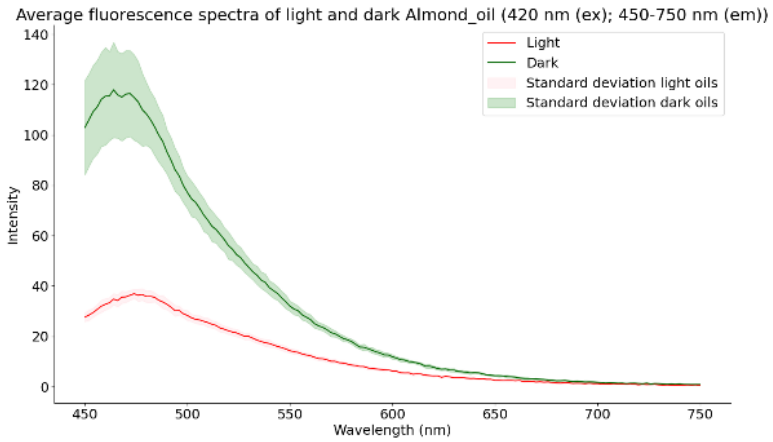

Light vs Dark Olive_oil_Poland
Dark
Light
Centre
Standard deviation
PC 2, explained variance 4.9%
PC 1, explained variance 92.8%

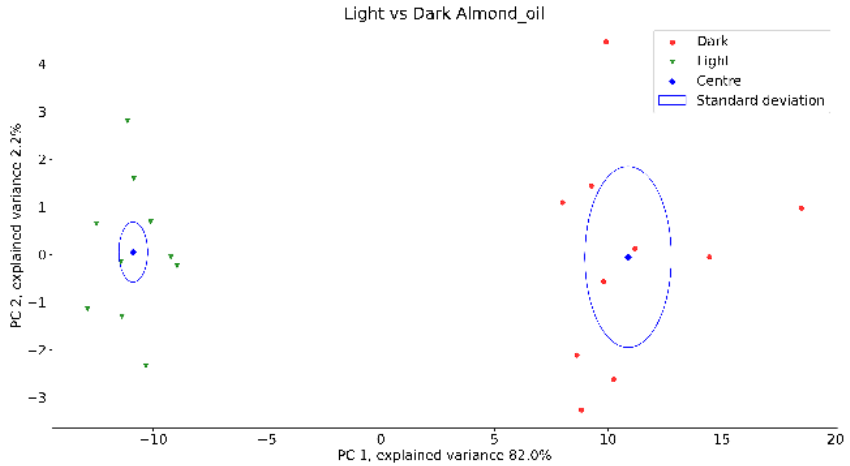

Average fluorescence spectra of light and dark White_bottle (380 nm (ex); 410-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

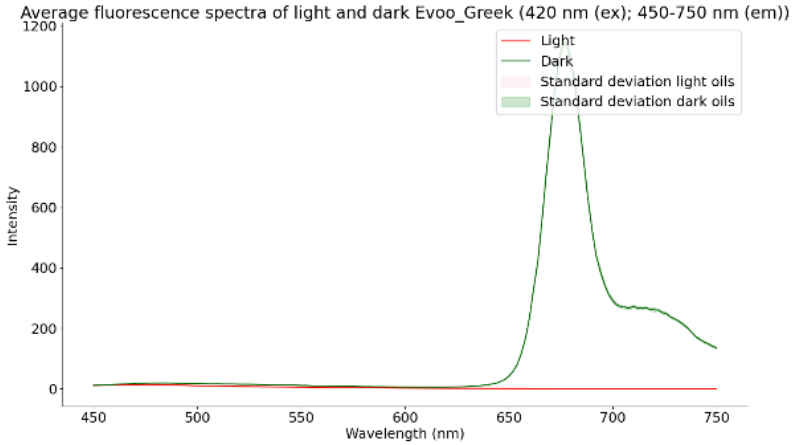

Light vs Dark White_bottle
Dark
Light
Centre
Standard deviation
PC 2, explained variance 13.4%
PC 1, explained variance 33.3%

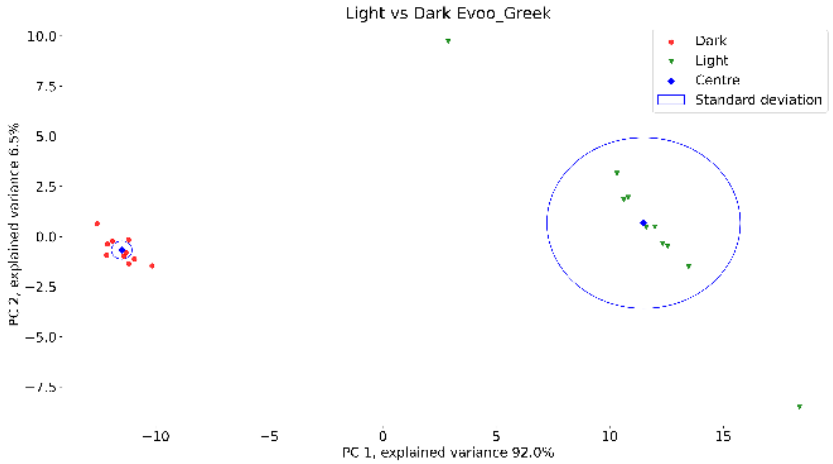
APPENDIX E

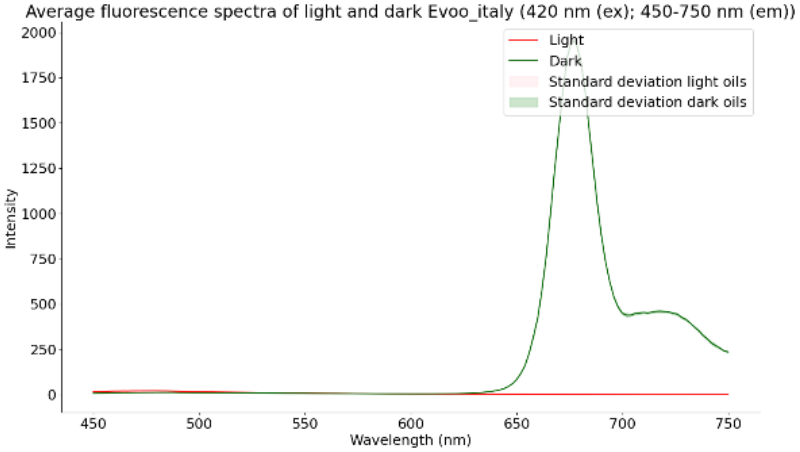
Figure E.1 - The results of analysis of Fluorescence (420 nm (ex), 450-750 nm (em)) oils data analysis and PCA visualization.

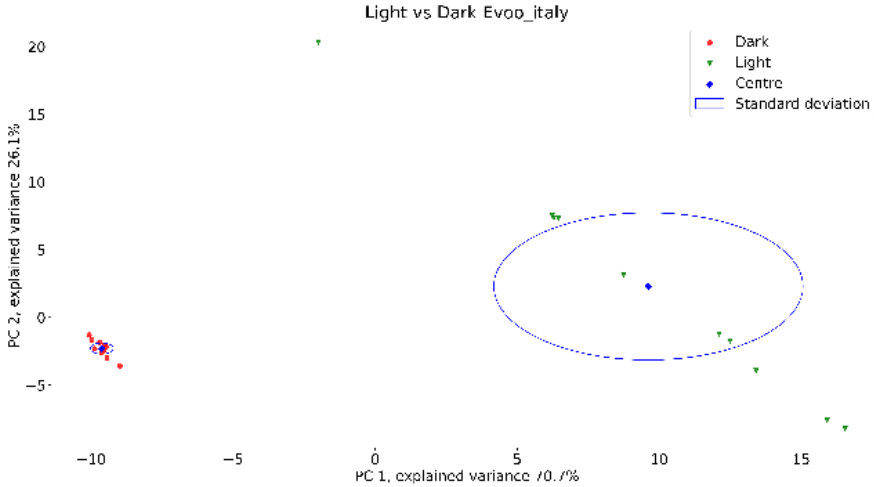


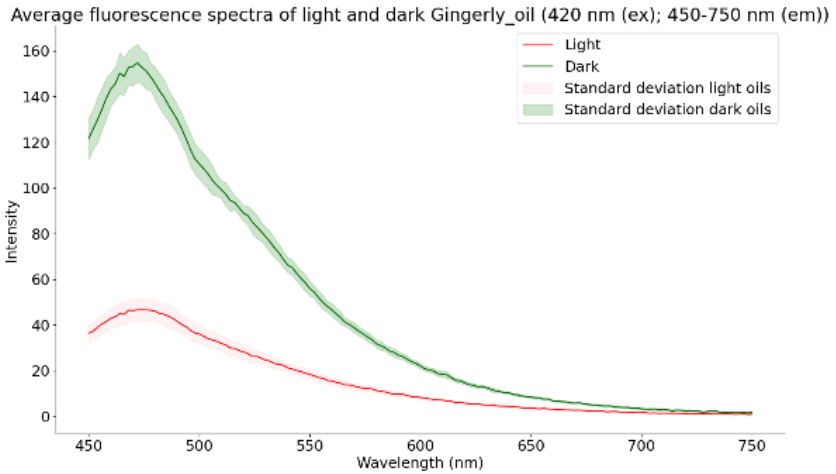


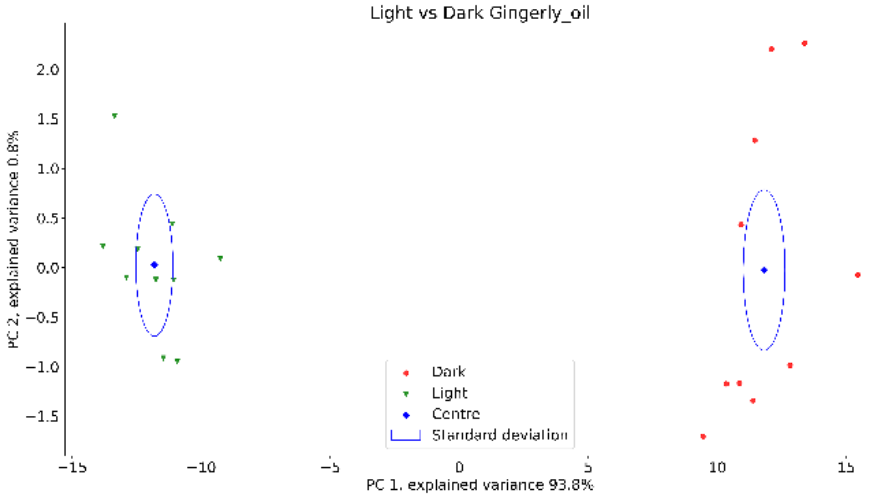

Average fluorescence spectra of light and dark Evoo_Greek (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

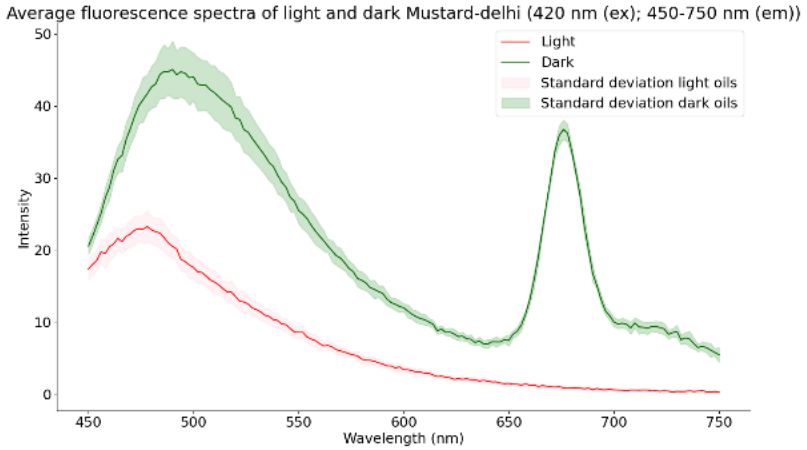

Light vs Dark Evoo_Greek
Dark
Light
Centre
Standard deviation
PC 2, explained variance 6.5%
PC 1, explained variance 92.0%

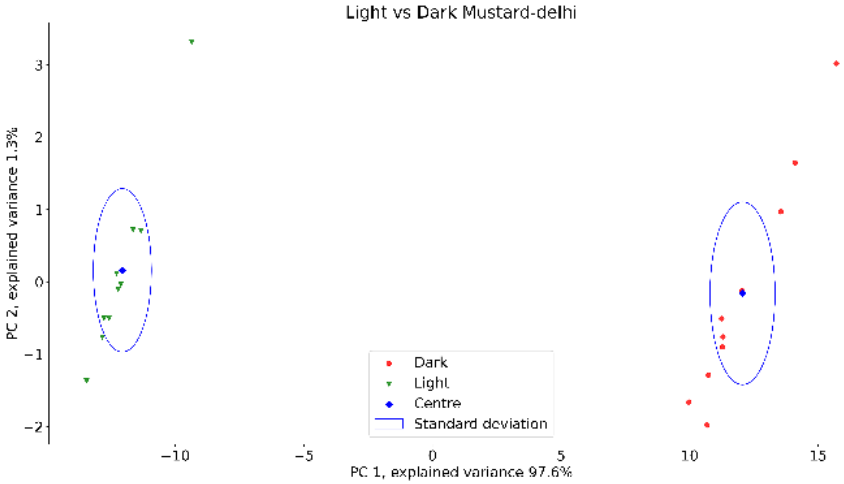

Average fluorescence spectra of light and dark Evoo_italy (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

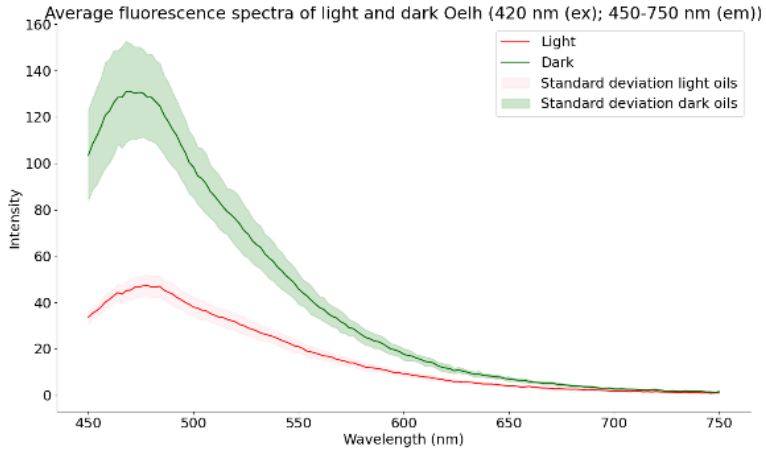

Light vs Dark Evoo_italy
Dark
Light
Centre
Standard deviation
PC 2, explained variance 26.1%
PC 1, explained variance 70.7%

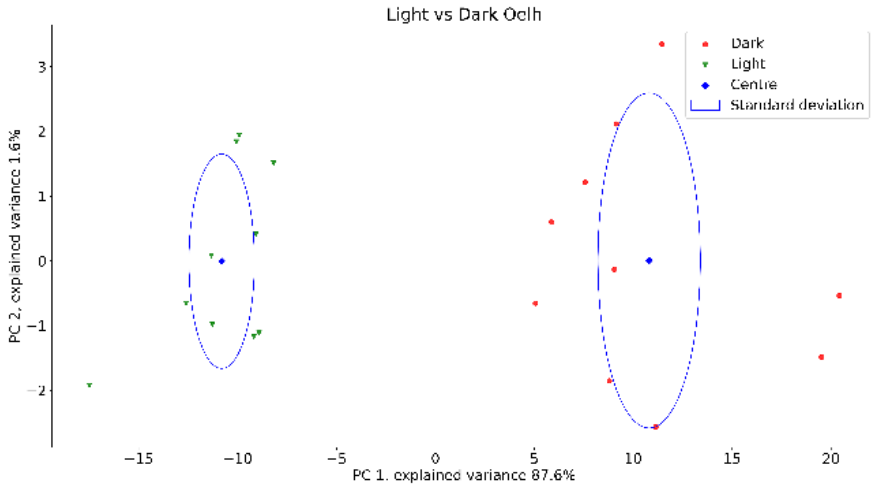

Average fluorescence spectra of light and dark Gingerly_oil (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

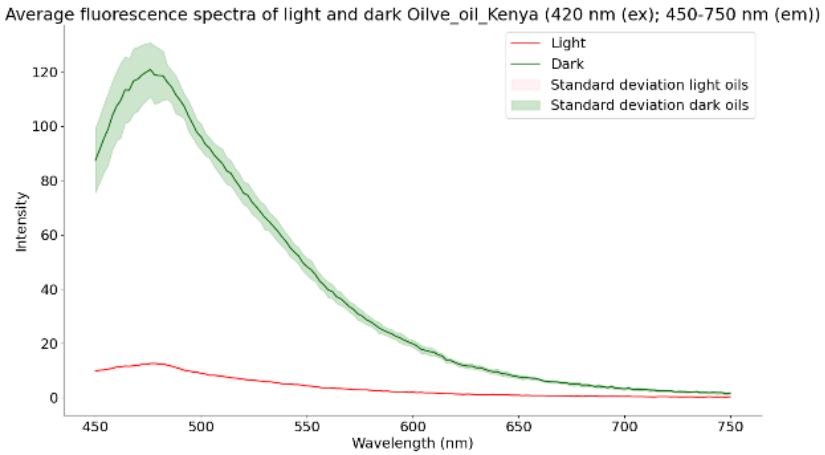

Light vs Dark Gingerly_oil
PC 2, explained variance 0.8%
PC 1, explained variance 93.8%
Dark
Light
Centre
Standard deviation

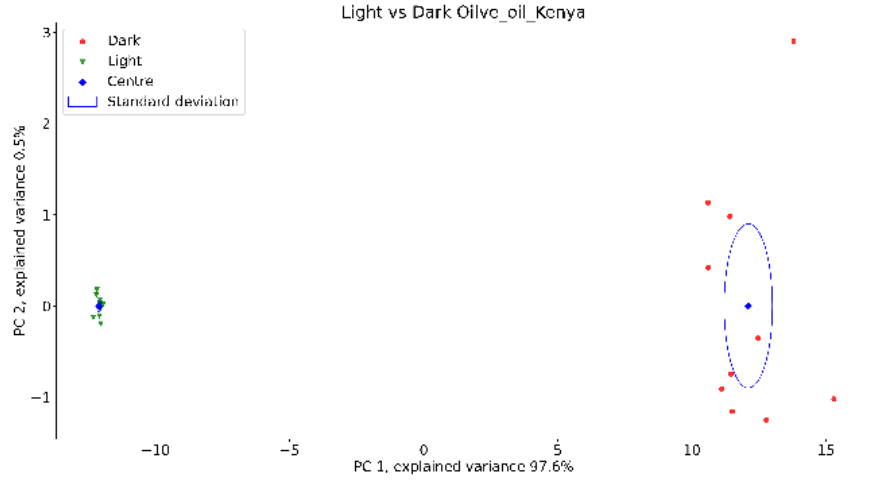

Average fluorescence spectra of light and dark Mustard-delhi (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

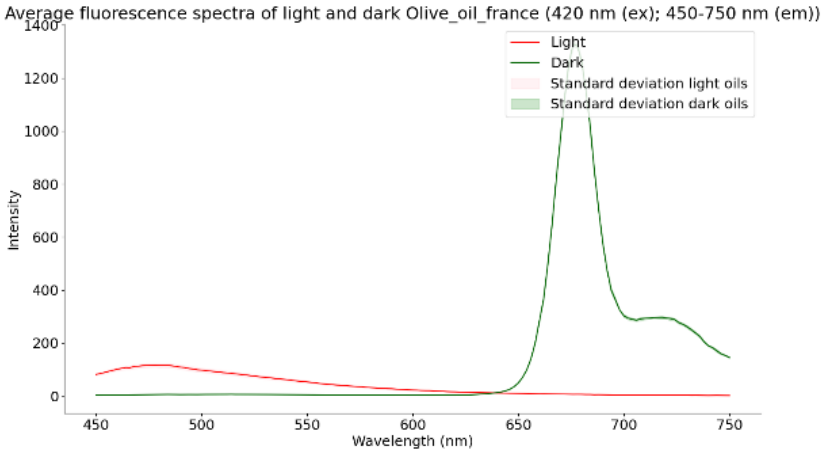

Light vs Dark Mustard-delhi
PC 2, explained variance 1.3%
PC 1, explained variance 97.6%
Dark
Light
Centre
Standard deviation

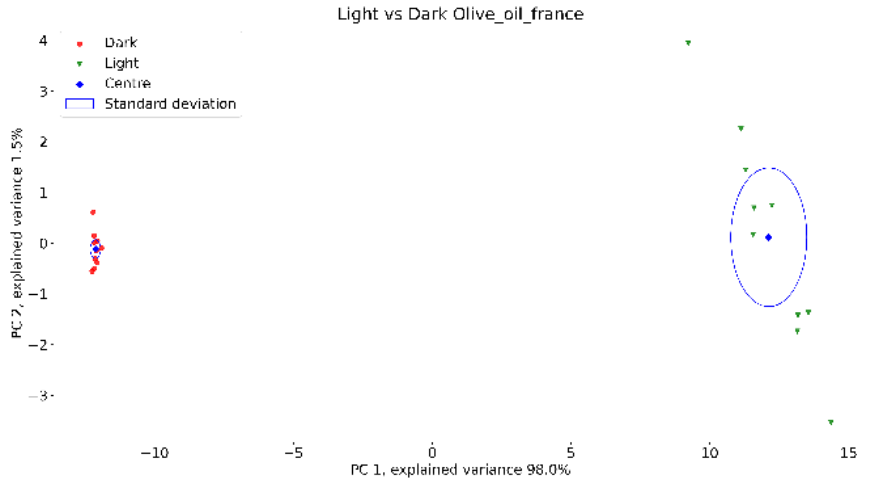

Average fluorescence spectra of light and dark Oelh (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

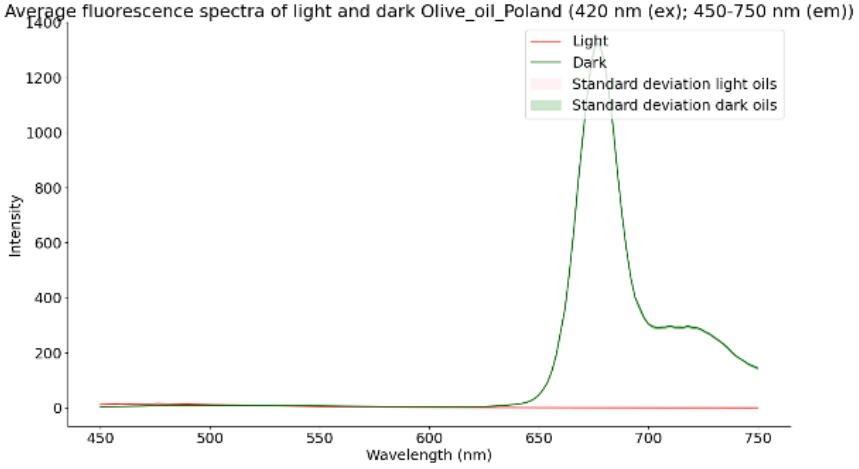

Light vs Dark Oelh
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.6%
PC 1, explained variance 87.6%

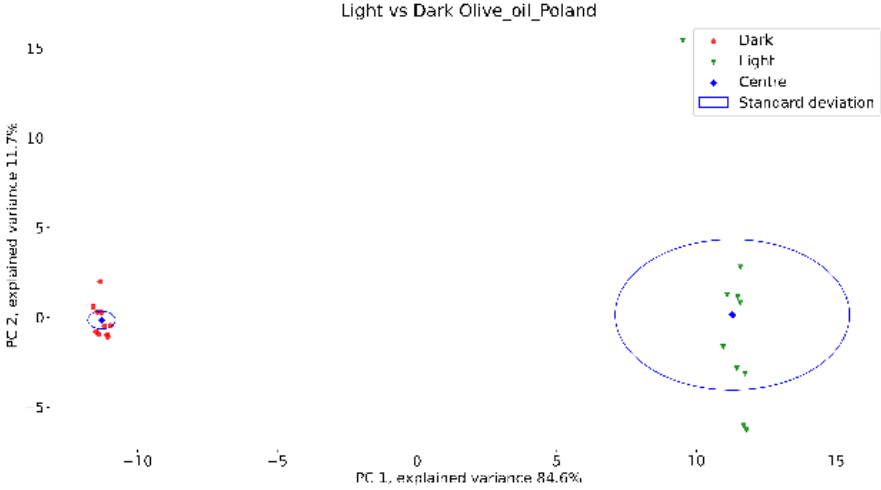

Average fluorescence spectra of light and dark Oilve_oil_Kenya (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

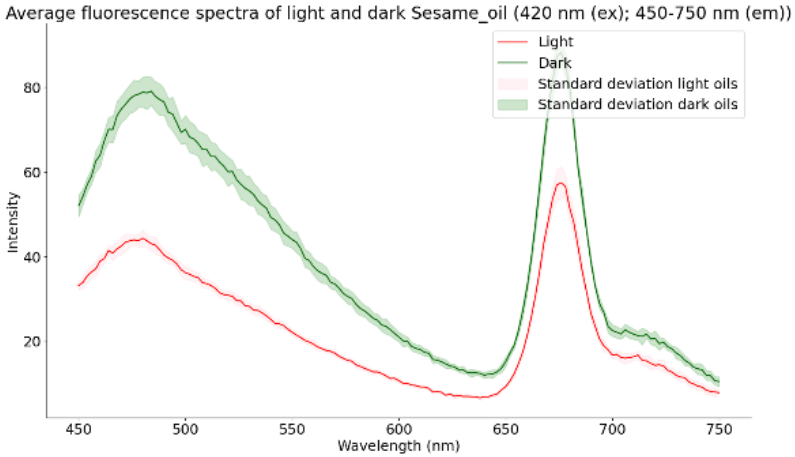

Light vs Dark Oilve_oil_Kenya
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.5%
PC 1, explained variance 97.6%

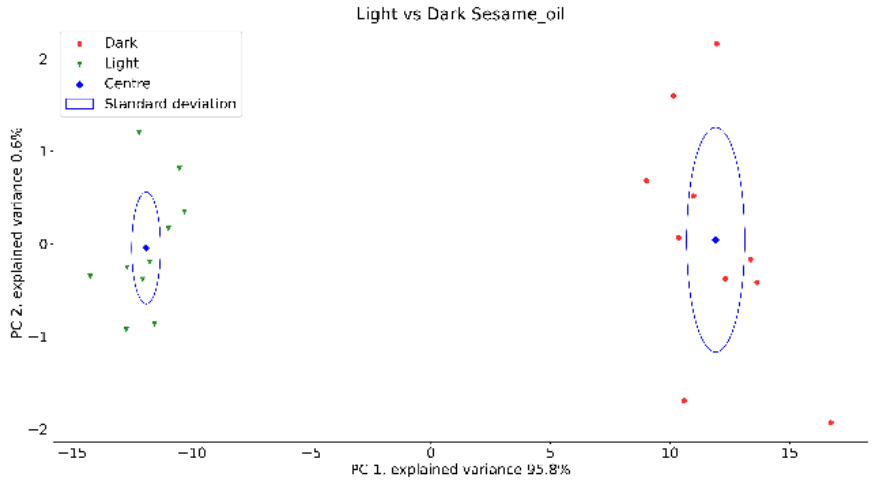

Average fluorescence spectra of light and dark Olive_oil_france (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

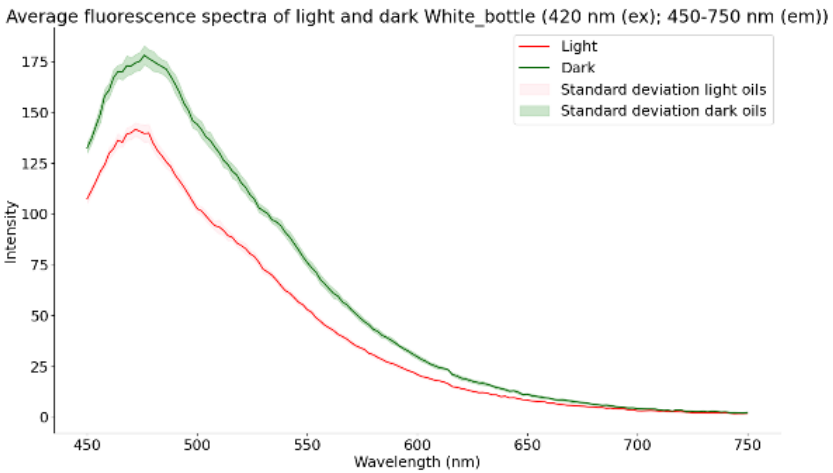

Light vs Dark Olive_oil_france
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.5%
PC 1, explained variance 98.0%

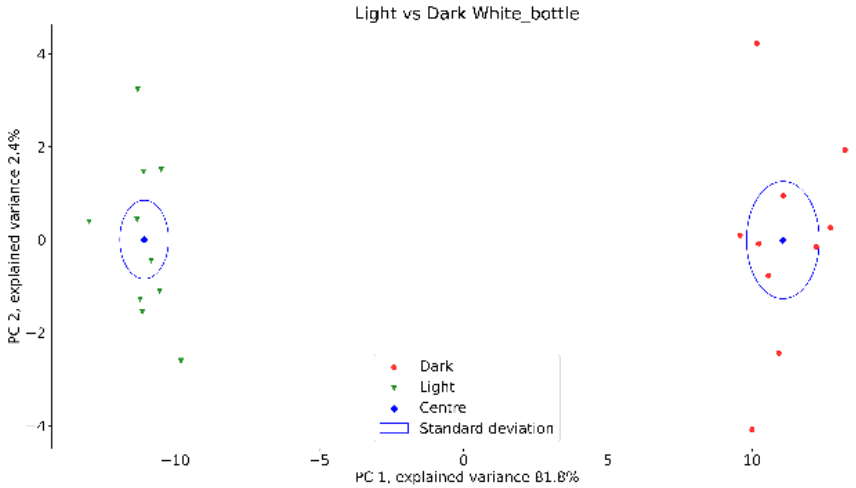

Average fluorescence spectra of light and dark Olive_oil_Poland (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)


Light vs Dark Olive_oil_Poland
Dark
Light
Centre
Standard deviation
PC 2, explained variance 11.7%
PC 1, explained variance 84.6%


Average fluorescence spectra of light and dark Sesame_oil (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

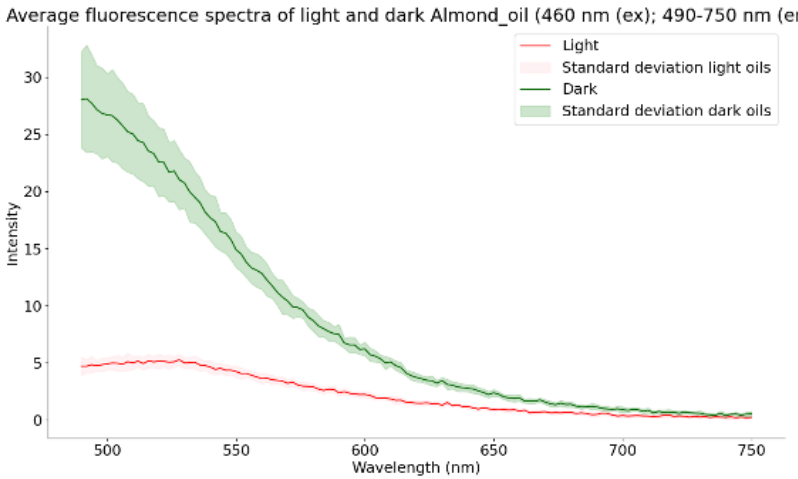

Light vs Dark Sesame_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.6%
PC 1, explained variance 95.8%

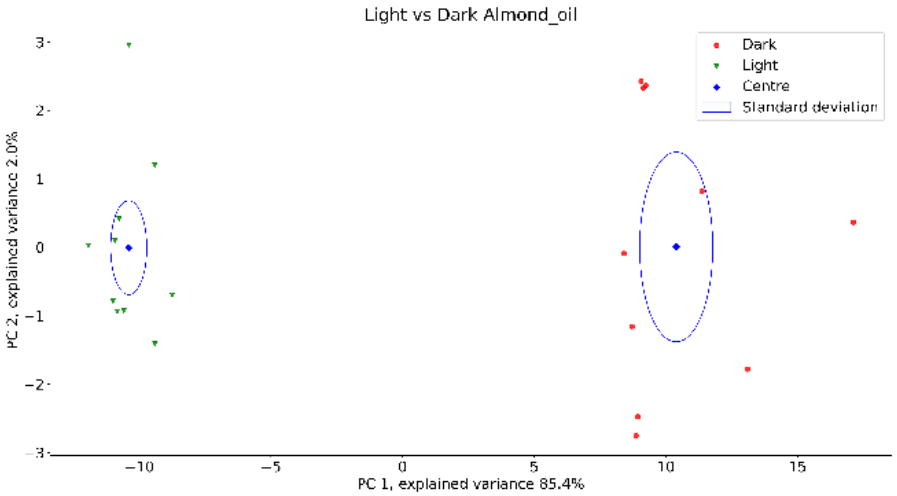

Average fluorescence spectra of light and dark White_bottle (420 nm (ex); 450-750 nm (em))
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
Wavelength (nm)

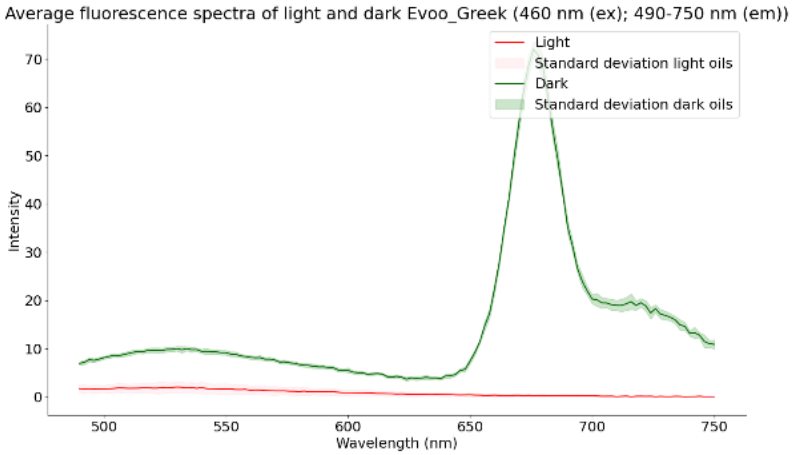

Light vs Dark White_bottle
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.4%
PC 1, explained variance 81.8%

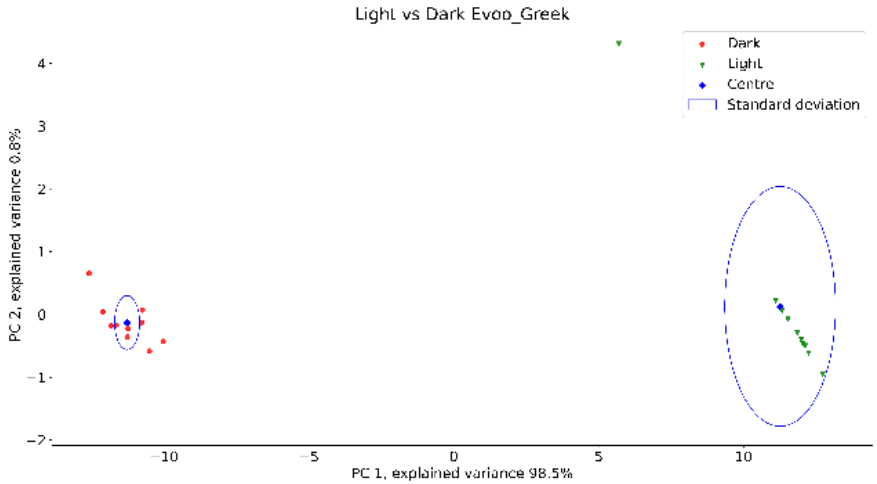
APPENDIX F

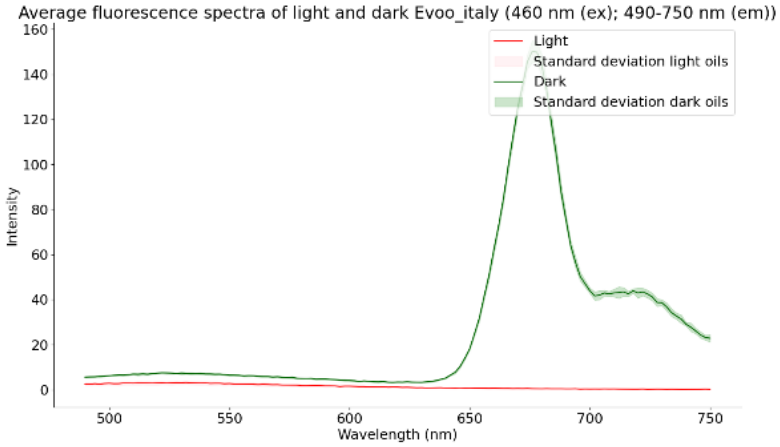
Figure F.1 - The results of analysis of Fluorescence (460 nm (ex), 490-750 nm (em)) oils data analysis and PCA visualization.

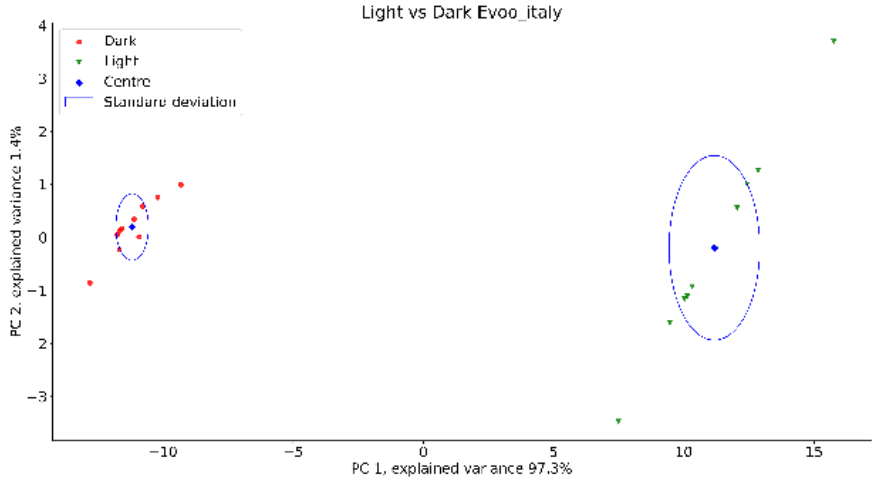


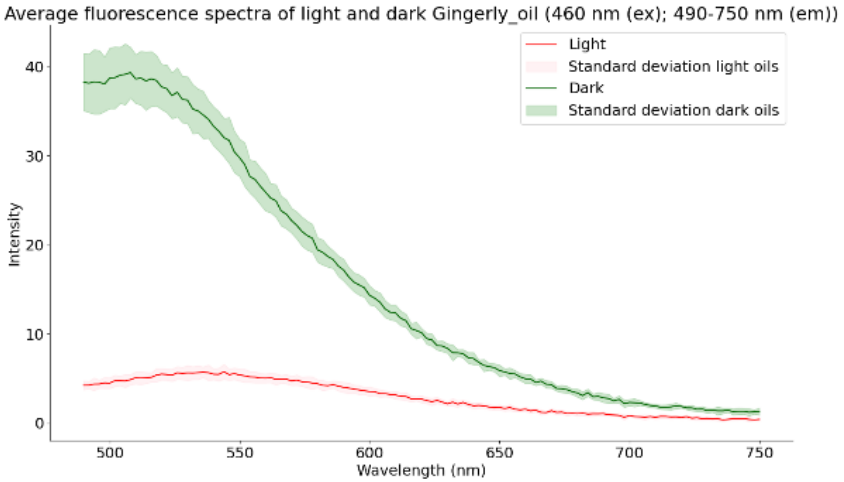


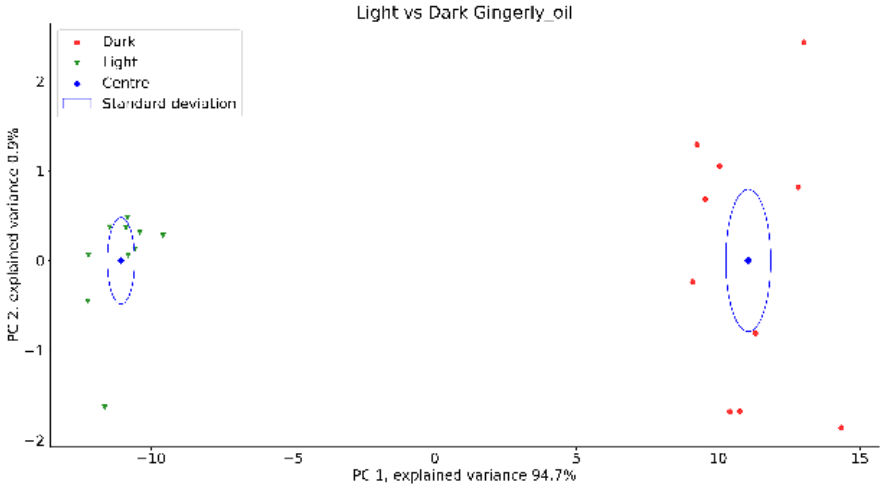

Average fluorescence spectra of light and dark Evoo_Greek (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

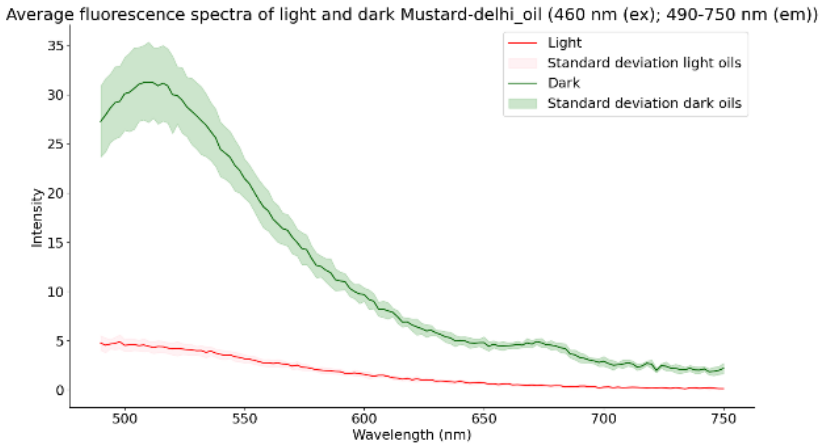

Light vs Dark Evoo_Greek
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.8%
PC 1, explained variance 98.5%

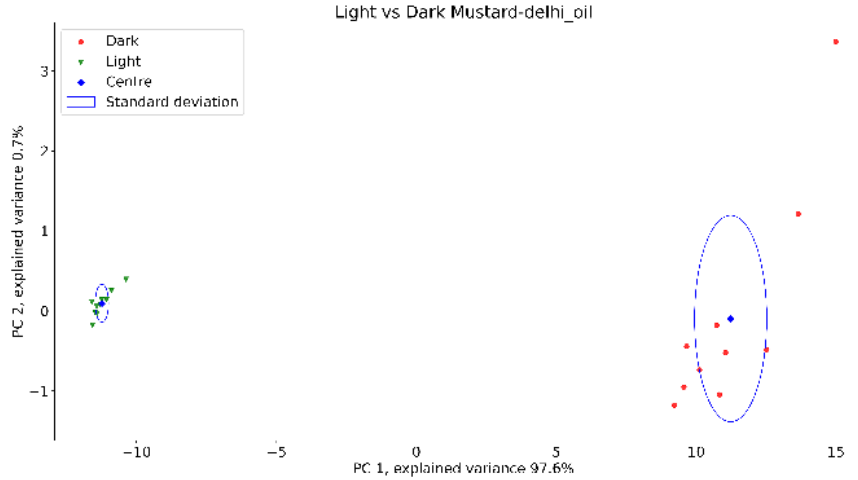

Average fluorescence spectra of light and dark Evoo_italy (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

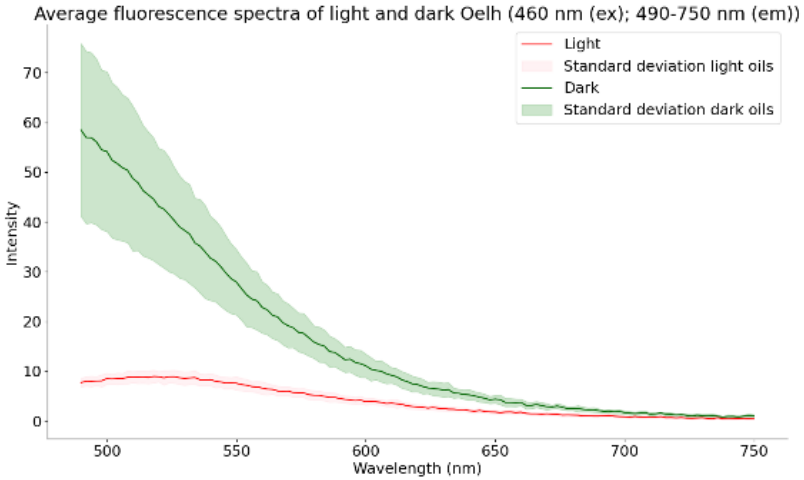

Light vs Dark Evoo_italy
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.4%
PC 1, explained variance 97.3%

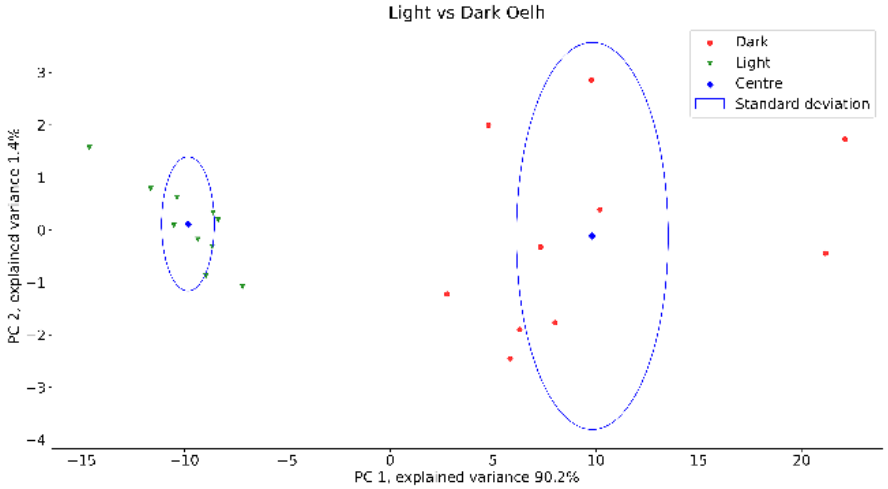

Average fluorescence spectra of light and dark Gingerly_oil (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

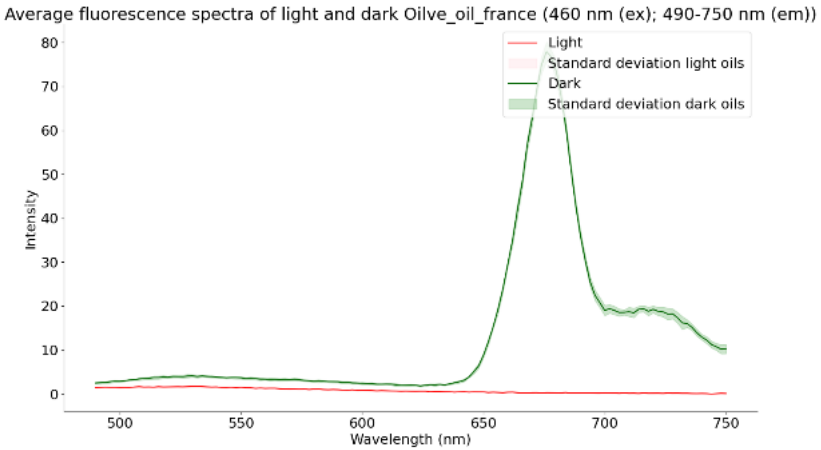

Light vs Dark Gingerly_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.9%
PC 1, explained variance 94.7%

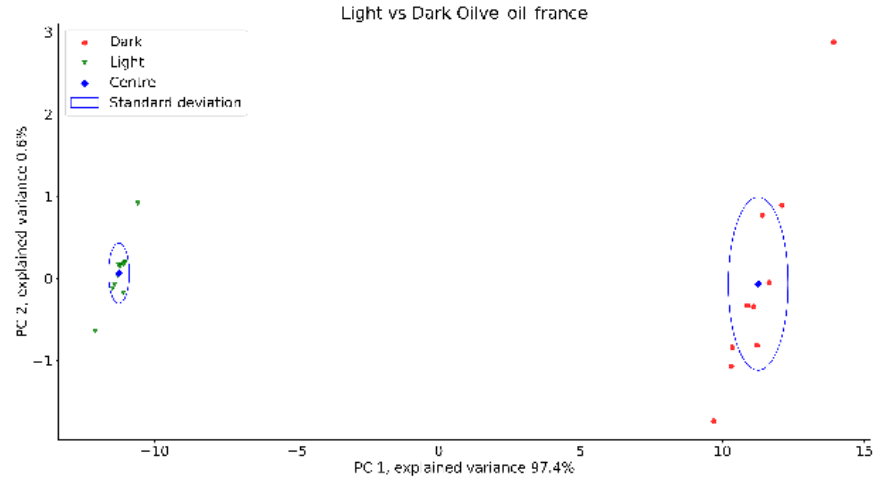

Average fluorescence spectra of light and dark Mustard-delhi_oil (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

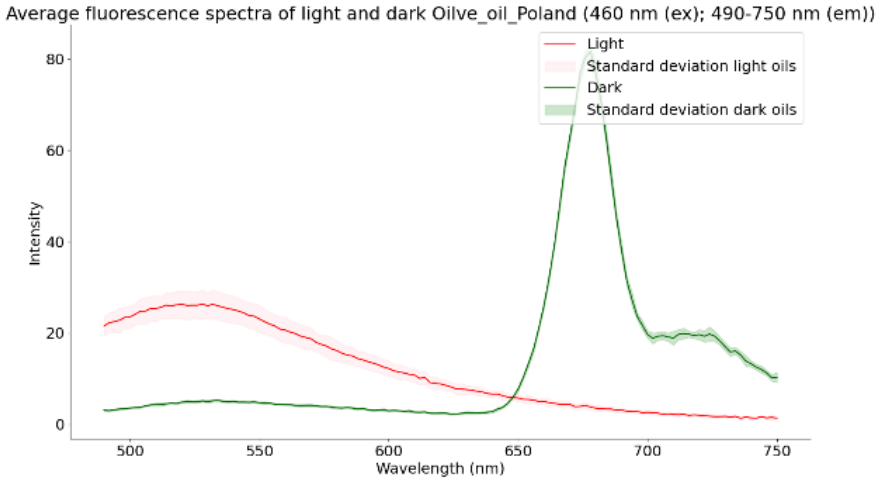

Light vs Dark Mustard-delhi_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.7%
PC 1, explained variance 97.6%

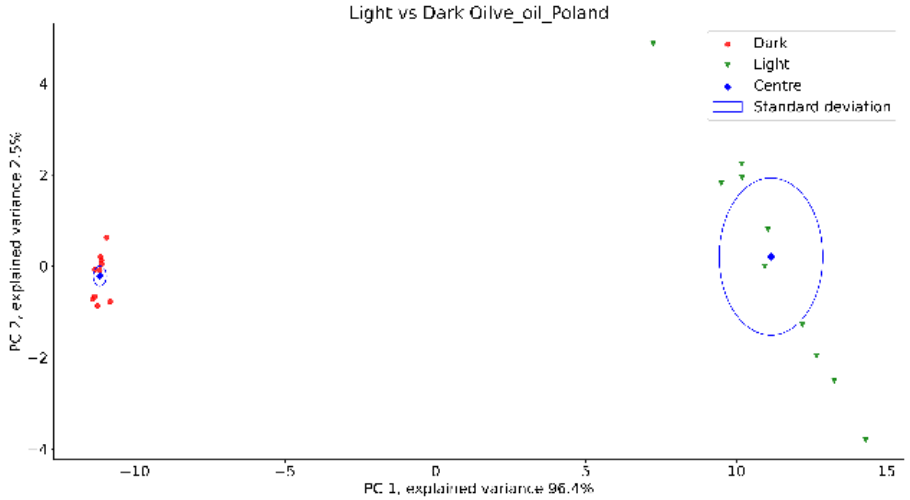

Average fluorescence spectra of light and dark Oelh (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

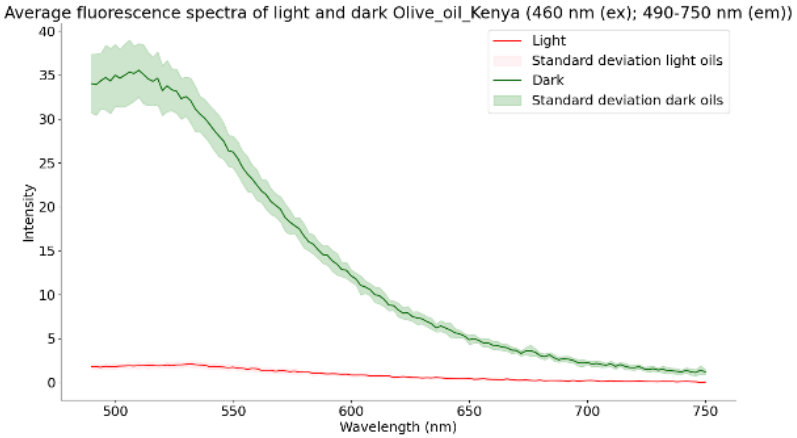

Light vs Dark Oelh
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.4%
PC 1, explained variance 90.2%

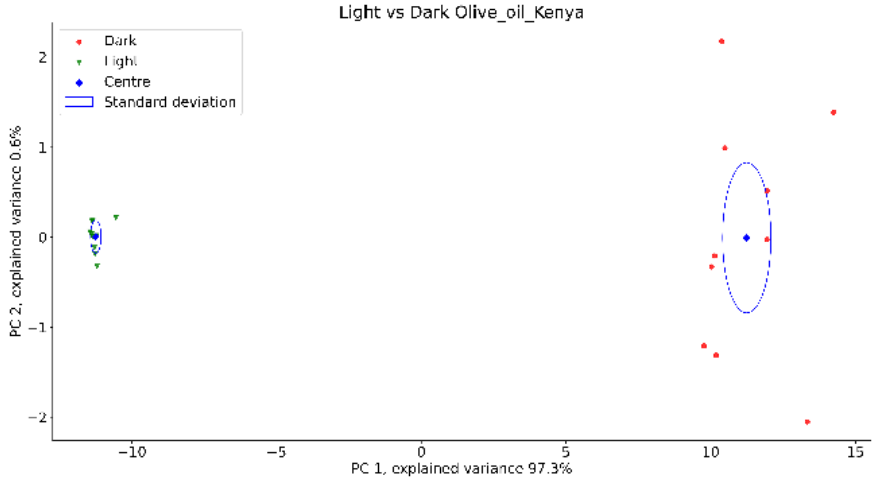

Average fluorescence spectra of light and dark Oilve_oil_france (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

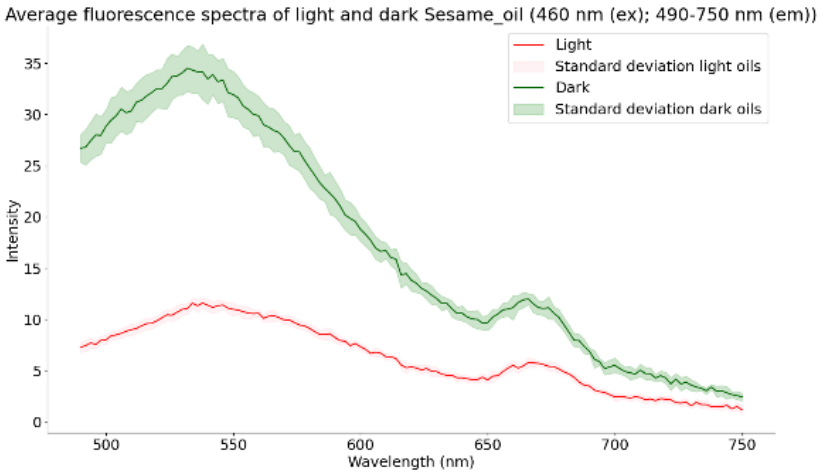

Light vs Dark Oilve oil france
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.6%
PC 1, explained variance 97.4%

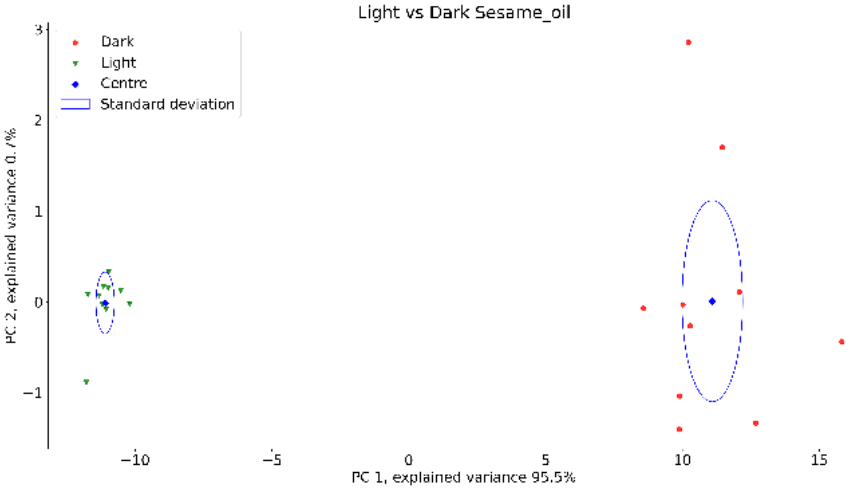

Average fluorescence spectra of light and dark Oilve_oil_Poland (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

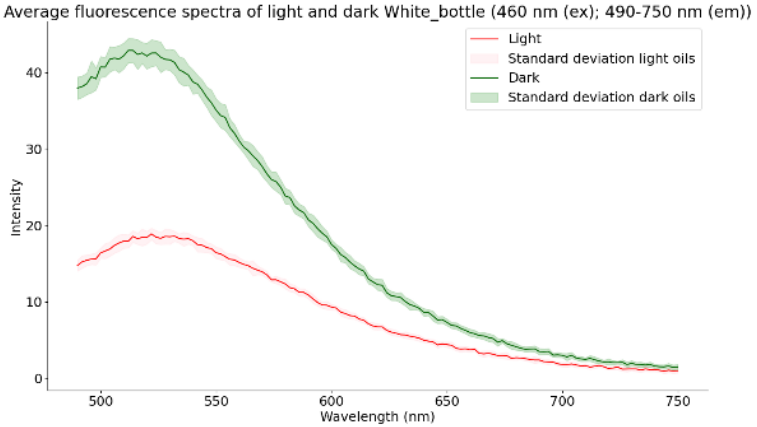

Light vs Dark Oilve_oil_Poland
Dark
Light
Centre
Standard deviation
PC 2, explained variance 2.5%
PC 1, explained variance 96.1%

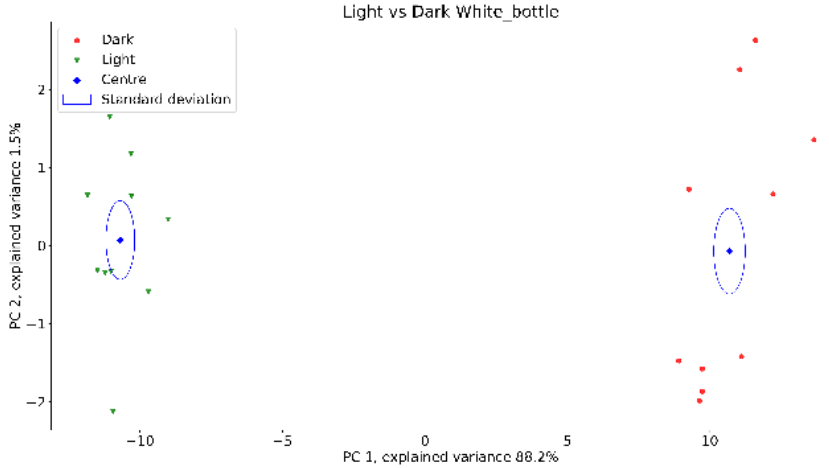

Average fluorescence spectra of light and dark Olive_oil_Kenya (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)


Light vs Dark Olive_oil_Kenya
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.6%
PC 1, explained variance 97.3%


Average fluorescence spectra of light and dark Sesame_oil (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

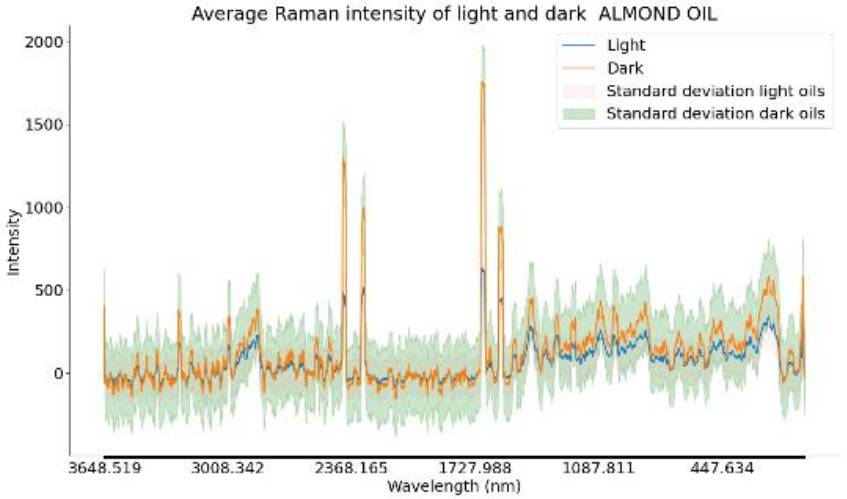

Light vs Dark Sesame_oil
Dark
Light
Centre
Standard deviation
PC 2, explained variance 0.7%
PC 1, explained variance 95.5%

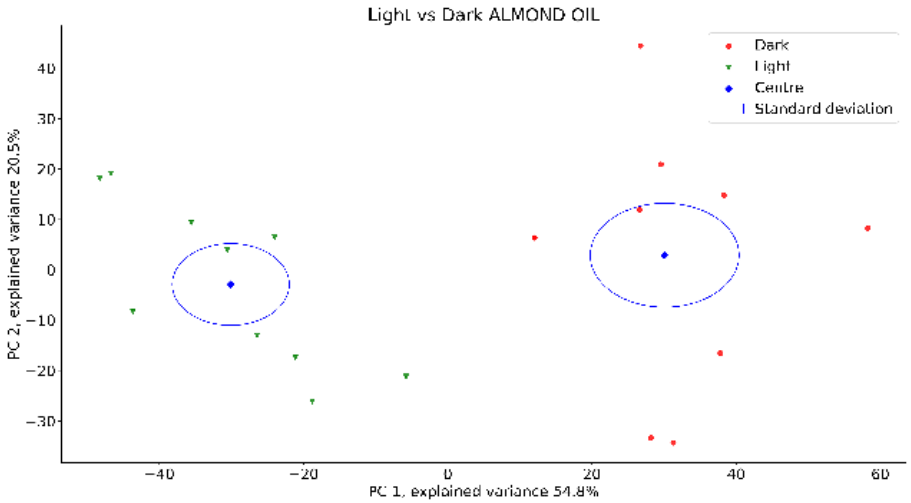

Average fluorescence spectra of light and dark White_bottle (460 nm (ex); 490-750 nm (em))
Light
Standard deviation light oils
Dark
Standard deviation dark oils
Intensity
Wavelength (nm)

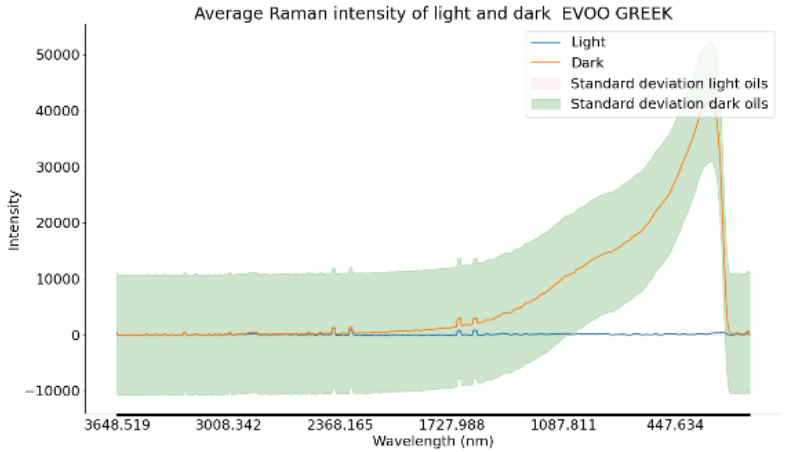

Light vs Dark White_bottle
Dark
Light
Centre
Standard deviation
PC 2, explained variance 1.5%
PC 1, explained variance 88.2%

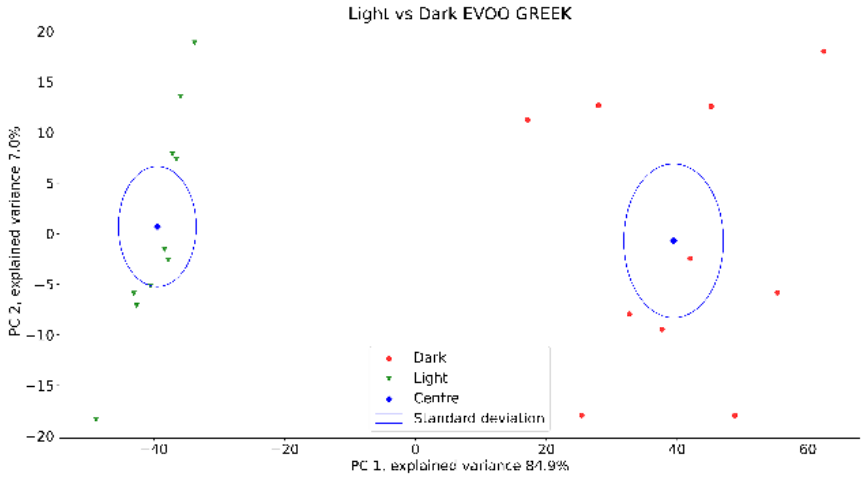
APPENDIX G

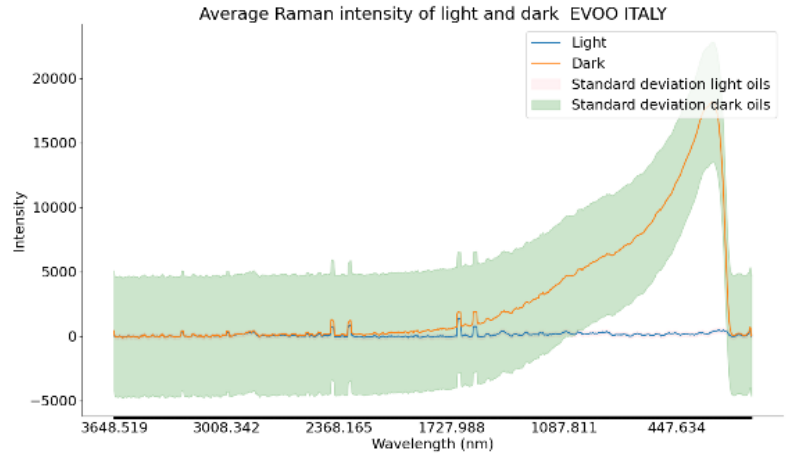
Figure G.1 - The results of analysis of Raman oils data analysis and PCA visualization.

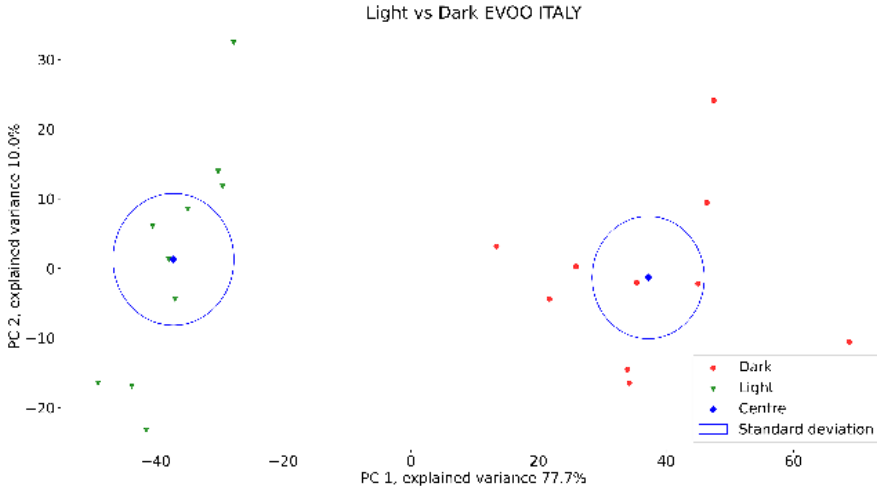


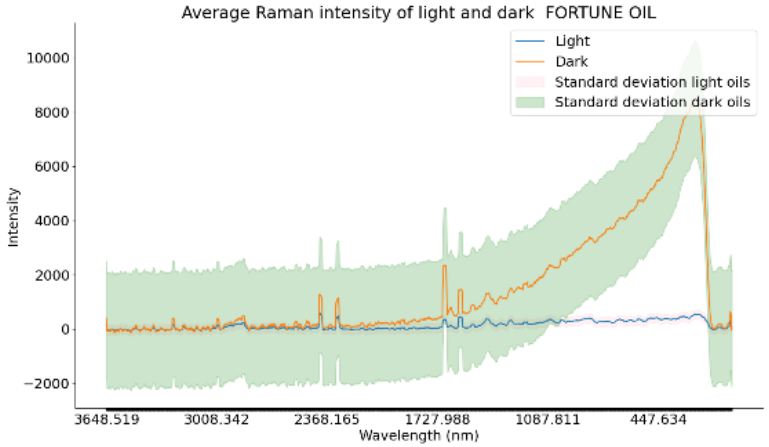


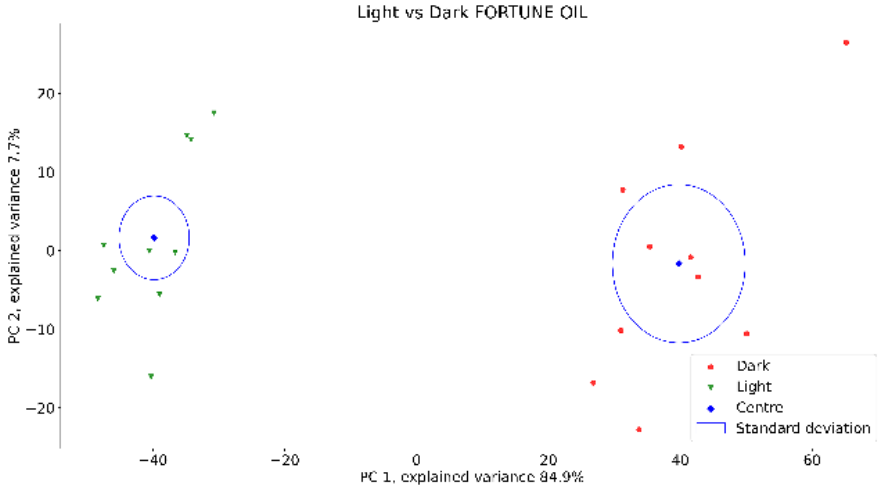

Average Raman intensity of light and dark EVOO GREEK
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
50000
40000
30000
20000
10000
0
−10000
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)

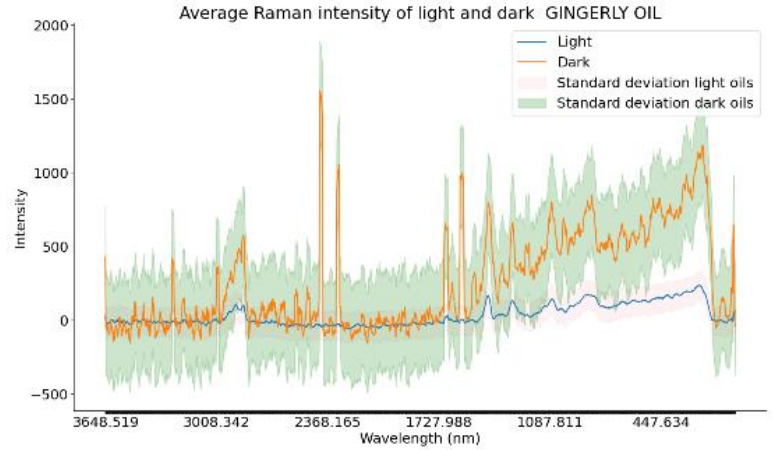

Light vs Dark EVOO GREEK
PC 2, explained variance 7.0%
20
15
10
5
0
−5
−10
−15
−20
−40
−20
0
20
40
60
PC 1, explained variance 84.9%
Dark
Light
Centre
Standard deviation

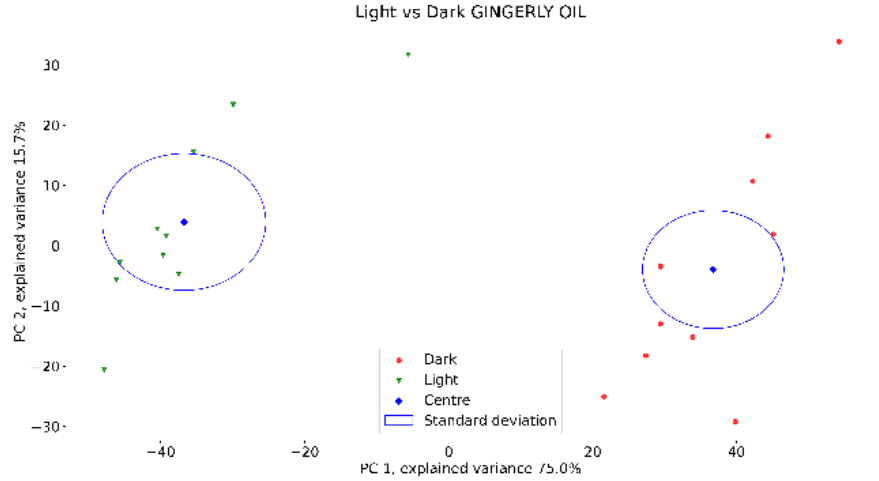

Average Raman intensity of light and dark EVOO ITALY
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
20000
15000
10000
5000
0
−5000
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)

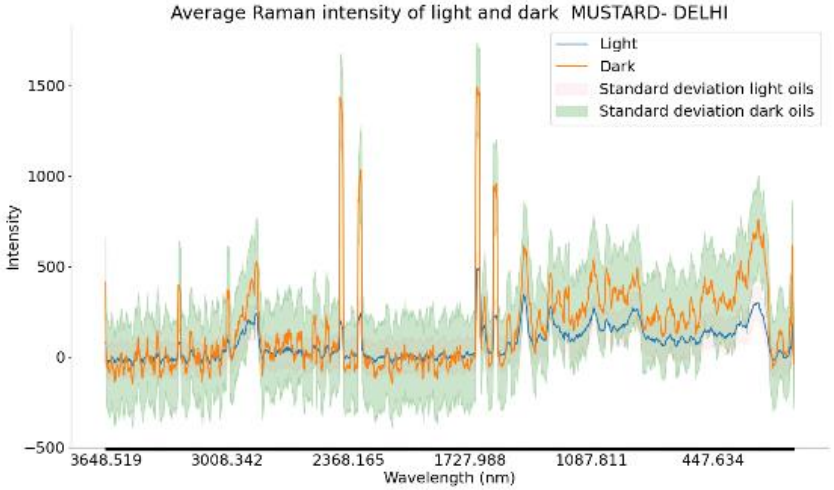

Light vs Dark EVOO ITALY
PC 2, explained variance 10.0%
30
20
10
0
−10
−20
−40
−20
0
20
40
60
PC 1, explained variance 77.7%
Dark
Light
Centre
Standard deviation

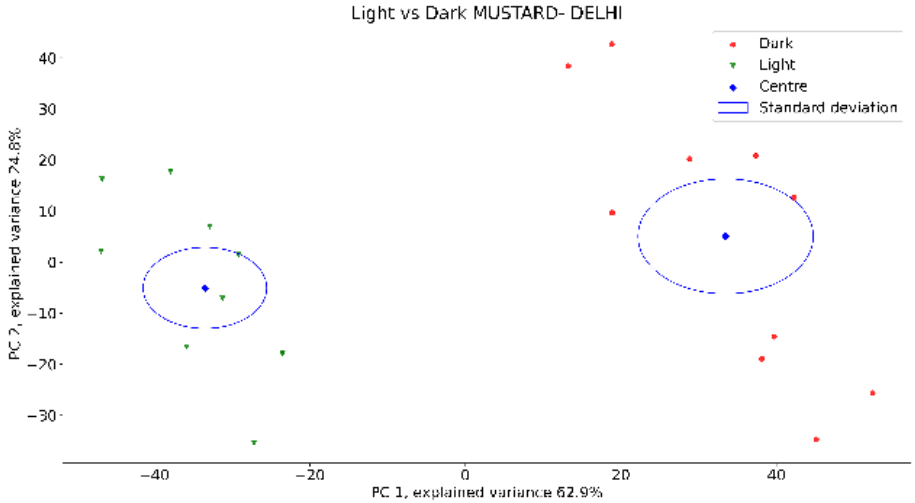

Average Raman intensity of light and dark FORTUNE OIL
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
10000
8000
6000
4000
2000
0
−2000
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)

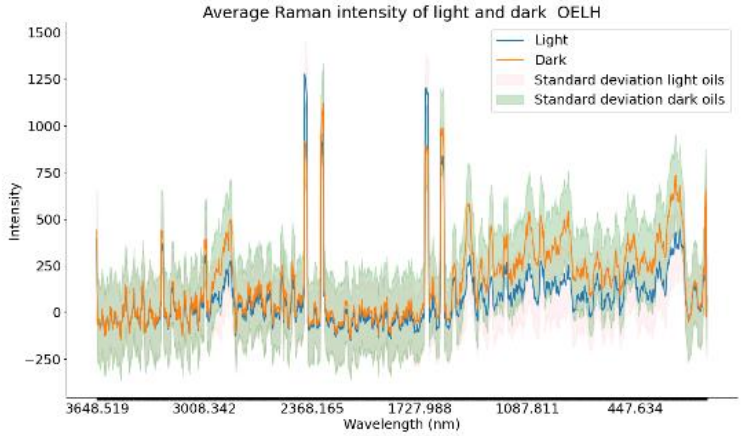

Light vs Dark FORTUNE OIL
PC 2, explained variance 7.7%
20
10
0
−10
−20
−40
−20
0
20
40
60
PC 1, explained variance 84.9%
Dark
Light
Centre
Standard deviation

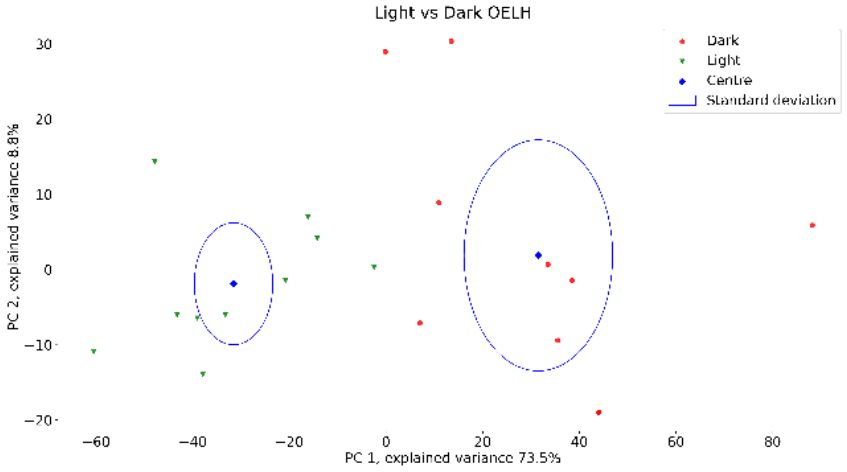

Average Raman intensity of light and dark GINGERLY OIL
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
2000
1500
1000
500
0
−500
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)

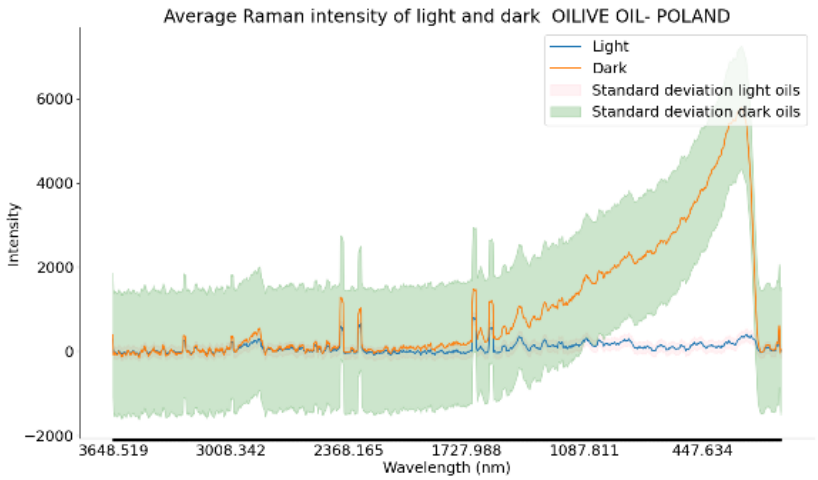

Light vs Dark GINGERLY OIL
PC 2, explained variance 15.7%
30
20
10
0
−10
−20
−30
−40
−20
0
20
40
PC 1, explained variance 75.0%
Dark
Light
Centre
Standard deviation

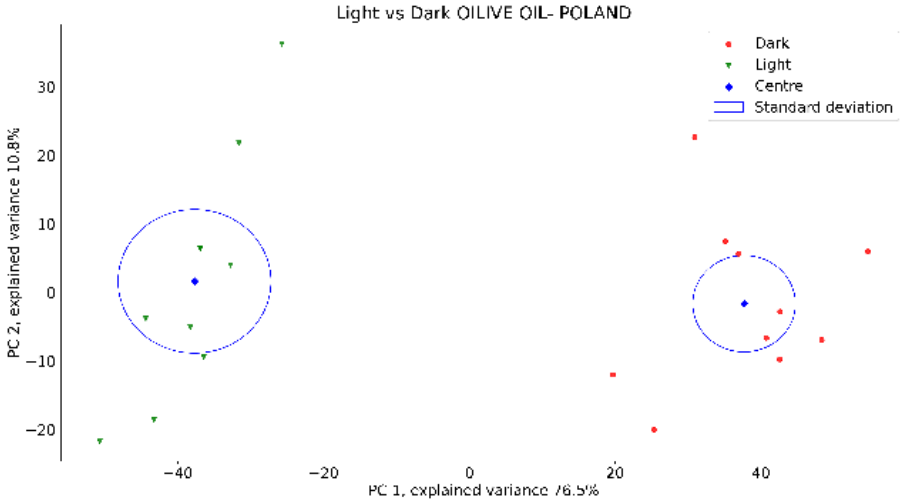

Average Raman intensity of light and dark MUSTARD- DELHI
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
1500
1000
500
0
−500
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)

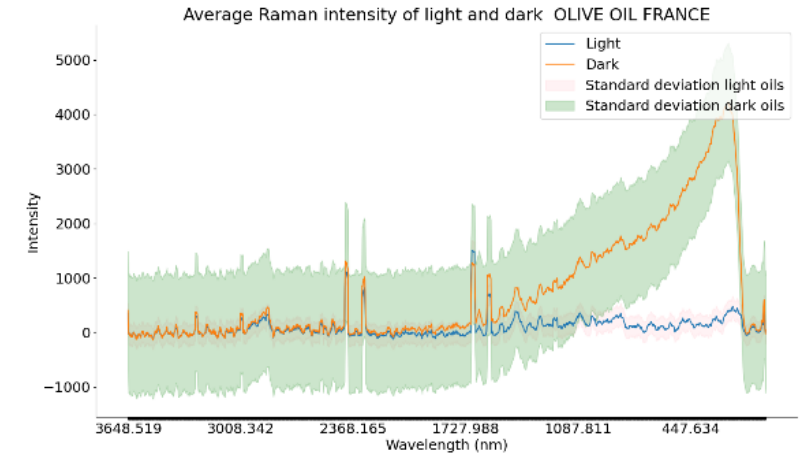

Light vs Dark MUSTARD- DELHI
Dark
Light
Centre
Standard deviation
PC 2, explained variance 24.8%
40
30
20
10
0
−10
−20
−30
−40
−20
0
20
40
PC 1, explained variance 62.9%

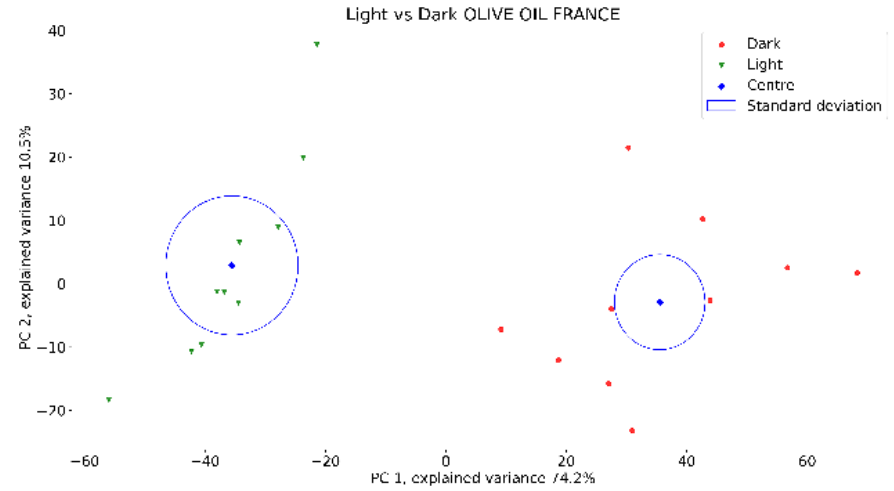

Average Raman intensity of light and dark OELH
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
1500
1250
1000
750
500
250
0
−250
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)

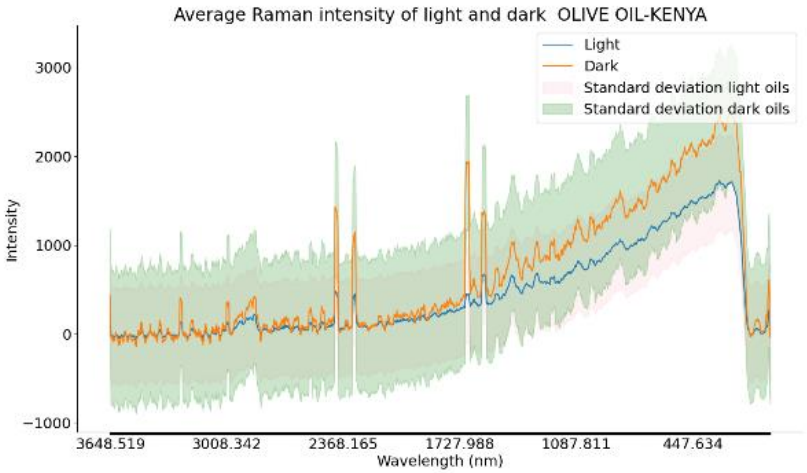

Light vs Dark OELH
Dark
Light
Centre
Standard deviation
PC 2, explained variance 8.8%
30
20
10
0
−10
−20
−60
−40
−20
0
20
40
60
80
PC 1, explained variance 73.5%

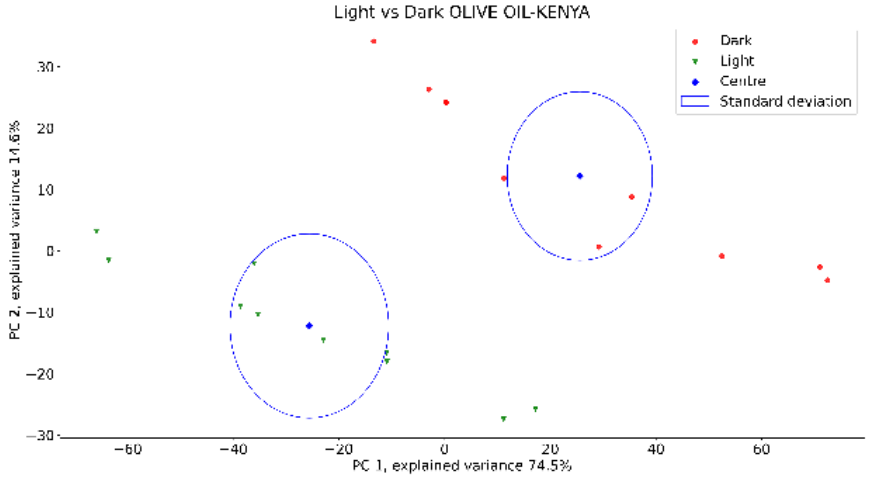

Average Raman intensity of light and dark OILIVE OIL- POLAND
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
6000
4000
2000
0
−2000
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)

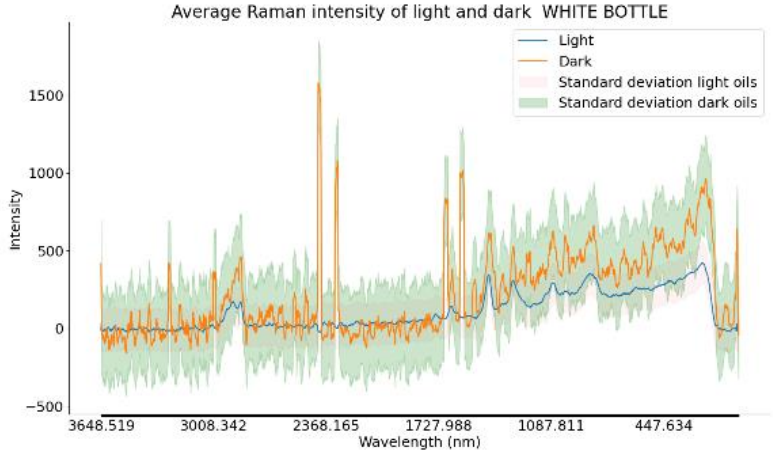

Light vs Dark OILIVE OIL- POLAND
Dark
Light
Centre
Standard deviation
PC 2, explained variance 10.8%
30
20
10
0
−10
−20
−40
−20
0
20
40
PC 1, explained variance 76.5%

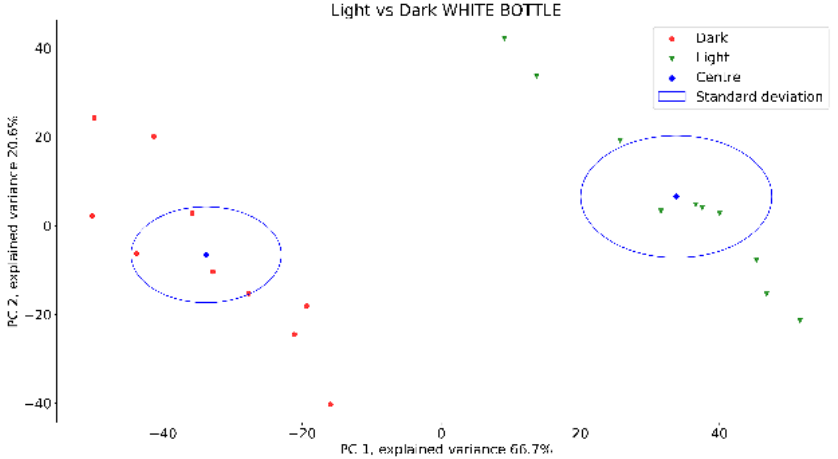

Average Raman intensity of light and dark OLIVE OIL FRANCE
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
5000
4000
3000
2000
1000
0
−1000
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)


Light vs Dark OLIVE OIL FRANCE
Dark
Light
Centre
Standard deviation
PC 2, explained variance 10.5%
40
30
20
10
0
−10
−20
−60
−40
−20
0
20
40
60
PC 1, explained variance 74.2%


Average Raman intensity of light and dark OLIVE OIL-KENYA
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
3000
2000
1000
0
−1000
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)


Light vs Dark OLIVE OIL-KENYA
Dark
Light
Centre
Standard deviation
PC 2, explained variance 14.6%
30
20
10
0
−10
−20
−30
−60
−40
−20
0
20
40
60
PC 1, explained variance 74.5%


Average Raman intensity of light and dark WHITE BOTTLE
Light
Dark
Standard deviation light oils
Standard deviation dark oils
Intensity
1500
1000
500
0
−500
3648.519
3008.342
2368.165
1727.988
1087.811
447.634
Wavelength (nm)


Light vs Dark WHITE BOTTLE
Dark
Light
Centre
Standard deviation
PC 2, explained variance 20.6%
40
20
0
−20
−40
−40
−20
0
20
40
PC 1, explained variance 66.7%

АНТИПЛАГИАТ
ОБНАРУЖЕНИЕ ЗАИМСТВОВАНИЙ

Отчет о проверке на заимствования №1

Автор: Воронова Гульнара Альфридовна
Проверяющий: Воронова Гульнара Альфридовна
Организация: Томский Государственный Университет

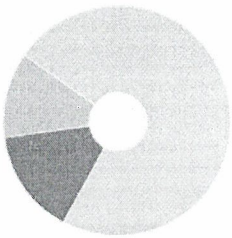
Отчет предоставлен сервисом «Антиплагиат» - http://tsu.antiplagiat.ru

ИНФОРМАЦИЯ О ДОКУМЕНТЕ

№ документа: 1
Начало загрузки: 07.06.2023 06:09:18
Длительность загрузки: 00:00:12
Имя исходного файла: Байцерова_Диплом.pdf
Название документа: Байцерова_Диплом
Размер текста: 76 кБ
Символов в тексте: 77228
Слов в тексте: 10843
Число предложений: 660

ИНФОРМАЦИЯ ОБ ОТЧЕТЕ

Начало проверки: 07.06.2023 06:09:31
Длительность проверки: 00:01:35
Комментарии: не указано
Поиск с учетом редактирования: да
Проверенные разделы: титульный лист с. 1, содержание с. 2-3, основная часть с. 4-44, библиография с. 45-49, приложение с. 50-92
Модули поиска: ИПС Адилет, Библиография, Сводная коллекция ЭБС, Интернет Плюс*, Сводная коллекция РГБ, Цитирование, Переводные заимствования (RuEn), Переводные заимствования по eLIBRARY.RU (EnRu), Переводные заимствования по коллекции Гарант: аналитика, Переводные заимствования по коллекции Интернет в английском сегменте, Переводные заимствования по Интернету (EnRu), Переводные заимствования по коллекции Интернет в русском сегменте, Переводные заимствования издательства Wiley , eLIBRARY.RU, СПС ГАРАНТ: аналитика, СПС ГАРАНТ: нормативно-правовая документация, Медицина, Диссертации НББ, Коллекция НБУ, Перефразирования по eLIBRARY.RU, Перефразирования по СПС ГАРАНТ: аналитика, Перефразирования по Интернету, Перефразирования по Интернету (EN), Перефразированные заимствования по коллекции Интернет в английском сегменте, Перефразированные заимствования по коллекции Интернет в русском сегменте, Перефразирования по коллекции издательства Wiley , Патенты СССР, РФ, СНГ, СМИ России и СНГ, Шаблонные фразы, Модуль поиска "tsu", Кольцо вузов, Издательство Wiley, Переводные заимствования



СОВПАДЕНИЯ	САМОЦИТИРОВАНИЯ	ЦИТИРОВАНИЯ	ОРИГИНАЛЬНОСТЬ
14,94%	0%	12,22%	72,84%

Совпадения — фрагменты проверяемого текста, полностью или частично сходные с найденными источниками, за исключением фрагментов, которые система отнесла к цитированию или самоцитированию. Показатель «Совпадения» – это доля фрагментов проверяемого текста, отнесенных к совпадениям, в общем объеме текста.

Самоцитирования — фрагменты проверяемого текста, совпадающие или почти совпадающие с фрагментом текста источника, автором или соавтором которого является автор проверяемого документа. Показатель «Самоцитирования» – это доля фрагментов текста, отнесенных к самоцитированию, в общем объеме текста.

Цитирования — фрагменты проверяемого текста, которые не являются авторскими, но которые система отнесла к корректно оформленным. К цитированиям относятся также шаблонные фразы; библиография; фрагменты текста, найденные модулем поиска «СПС Гарант: нормативно-правовая документация». Показатель «Цитирования» – это доля фрагментов проверяемого текста, отнесенных к цитированию, в общем объеме текста.

Текстовое пересечение — фрагмент текста проверяемого документа, совпадающий или почти совпадающий с фрагментом текста источника.

Источник — документ, проиндексированный в системе и содержащийся в модуле поиска, по которому проводится проверка.

Оригинальный текст — фрагменты проверяемого текста, не обнаруженные ни в одном источнике и не отмеченные ни одним из модулей поиска. Показатель «Оригинальность» – это доля фрагментов проверяемого текста, отнесенных к оригинальному тексту, в общем объеме текста.

«Совпадения», «Цитирования», «Самоцитирования», «Оригинальность» являются отдельными показателями, отображаются в процентах и в сумме дают 100%, что соответствует полному тексту проверяемого документа.

Обращаем Ваше внимание, что система находит текстовые совпадения проверяемого документа с проиндексированными в системе источниками. При этом система является вспомогательным инструментом, определение корректности и правомерности совпадений или цитирований, а также авторства текстовых фрагментов проверяемого документа остается в компетенции проверяющего.

С отчетом ознакомлен, научный руководитель, д-р ф-м н. профессор
Н.В. Клетенев
07.06.23

№	Доля в тексте	Доля в отчете	Источник	Актуален на	Модуль поиска	Комментарии
[01]	12,22%	12,22%	не указано	29 Сен 2022	Библиография	
[02]	2,95%	2,95%	A Study on Structural Optical and Electrical Properties ... https://shodhganga.inflibnet.ac.in	11 Дек 2022	Перефразированные заимствования по коллекции Интернет в английском сегменте	
[03]	2,58%	2,58%	https://mdpi-res.com/d_attachment/molecules/molec... https://mdpi-res.com	25 Янв 2023	Перефразированные заимствования по коллекции Интернет в английском сегменте	
[04]	2,52%	1,73%	UV-Vis Spectroscopy: Principle, Strengths and Limitatio... https://technologynetworks.com	25 Июн 2022	Интернет Плюс*	
[05]	2,02%	1,11%	http://www.ijitee.org/wp-content/uploads/Souvenir_V... http://ijitee.org	26 Мар 2020	Интернет Плюс*	
[06]	2,01%	0,41%	A Study on Structural Optical and Electrical Properties ... https://shodhganga.inflibnet.ac.in	11 Дек 2022	Интернет Плюс*	
[07]	1,66%	0,05%	Machine learning - Wikipedia https://en.wikipedia.org	30 Мая 2023	Интернет Плюс*	