SpMap: Hyperspectral package for spectroscopists in Python 3 Technical Document

Version 0.5

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Contents

List of Code Listings

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1 Introduction

Hyperspectral imaging offers new applications in agriculture, pharmaceutical, space, food, and many upcoming applications such as medical diagnosis. The analysis of hyperspectral images requires advanced software for processing thousands of bands in the image. The forthcoming developments related to fast hyperspectral imaging, automation and deep learning applications demand innovative software developments. This manual presents a new package based on Python 3 for spectroscopists and enthusiasts for developing new applications in hyperspectral imaging. The package is defined as SpectraMap(SpMap).

SpMap is a python package for high level hyperspectral data processing and scripting. The type of datasets can be any optical spectroscopic data with intensity and wavenumber axes. For example, infrarred and Raman spectroscopies.

The upcoming content shows how to handle data from an imaging spectroscopic point of view rather pure programming and developing approach. A high-level programming software offers a short scripting structure for fast and efficient hyperspectral data analysis. SpMap comes with several and research dataset-examples for understanding and practicing the tools implemented in SpMap.

The Table 1 shows examples to explore and use the tools in SpMap. A complete information regarding SpMap methods are shown throughout this manual.For the data related to the examples visit examples.

1.1 Hyperspectral object structure

Fig. 1 shows the hyperspectral data object structure that is established in the SpMap package. The object holds an index and columns along x-axis or wavenumber. The rows contain the Raman intensity (Fig. 6a). Datasets

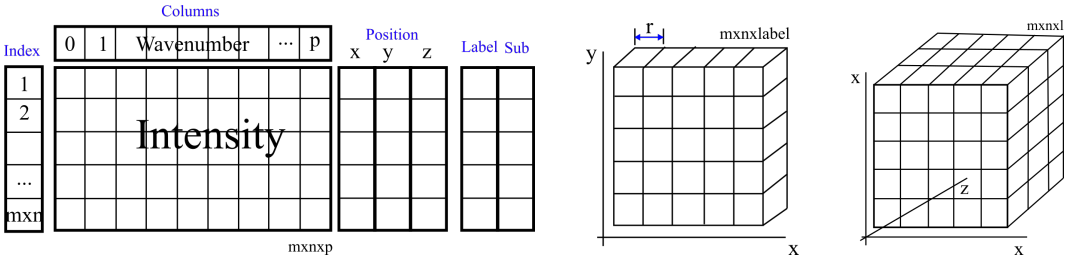
Table 1: Examples in SpMap

No.	Example	Description	Page
1	Raman spectra of plastics	Read CSV file, baseline correction and visualization of Raman data.	11
2	Depth profiling of multilayer of plastics	Read CSV, preprocessing and depth profile analysis of Raman data.	
3	Microplastics in tissue	Detectino of microplastics in tissue.	
4	3D Raman hyperspectral image	Detection of microplastics in tissue by 3D analysis.	
5	Tumor in bladder sections	Segmentation of biomolecues.	
6	Infrarred hyperspectral image	Analysis of an infrarred image.	
7	3D hyperspectral image	Detection of Microplastics in a volumetric image.	
8	Hyperspectral images of bladder	Pre and processing of bladder Raman images	
9	Plastics: unmixing by PCA and PLS-LDA	Separation of plastics by principal components and linear-discriminant analysis	

from 2D or 3D imaging provide spatial information represented as x, y and z in the position table of every pixel. The label is associated to the naming and meaning of every pixel. Sublabel offers an extra labeling useful for plotting and tracking changes. Confocal Raman microscopy supplies also z or depth information to plot 3D images Fig.1c .

1.2 Python and installation of SpMap

The predetermined work interface is Python 3. For further information concerning how to install the necessary requirements, visit the link SpMap PyPi. The required external libraries are: Scikit-Learn [1], standard libraries: matplotlib, NumPy and pandas, besides complex algorithms: vertex component analysis [3], alternative iterative reweighted penalized least



(a) (b) (c)

Figure 1: Hyperspectral Object, (a) visual representation, (b) 2D map, (c) 3D volume

squares [4] and hierarchical density based clustering with applications with noise HDBSCAN [2]. After the installation of SpMap, we can import SpMap in Python:

```
# importing SpMap library in python
from spectramap import spmap as sp
```

1.3 SpMap hyperobject, methods and attributes

SpMap is based on dataframe structure (Fig. 6a) that contains attributes for containing the data of intensities, wavenumber, label and positions and methods for reading, manipulation, preprocessing, processing, and visualization of hyperspectral data. Visit the link: https://github.com/spectramap/spectramap for further information and to find examples.

1.4 Basic Data Handling methods

1.4.1 Creating/Deleting an SpMap object

The hyper object can contain any kind of data, spc, csv, txt or custom if it keeps the standard dataframe shape (Fig. 6a). The next command lines show how to create and delete the hyperobjects:

```
# creating an hyperobject called name in the variable mapa
mapa = sp.hyper_object('name')

# deleting mapa hyperobject
del mapa
```

1.4.2 Reading/saving csv, spc, mat and any common file

Some standard data files are spc, csv and txt, the next lines show some reading methods. The variable path may be the directory path and name for single readings and for multi readings path is the directory file of the datasets.

```
# Reading single spc file
mapa.read_single_spc(path)
# Reading several spc files
mapa.read_multi_spc(path)
# CSV (standard file in SpMap)
mapa.read_csv(path)
# compressed CSV (standard file in SpMap)
mapa.read_csv_xz(path)
# Any file (custom reading) (see coming example)
pandas.read_table(parameters)
# Mat (read a raw Mat) (require custom reading)
mat = read_mat(path)
# Show spectral data, average and individual
mapa.show(True), mapa.show(False)
# Save spectral data (CSV)
mapa.save_data(path, 'name')
# Save compressed spectral data (CSV_xz)
mapa.save_data_xz(path, 'name')
```

1.4.3 Other methods

This section provides methods for data manipulation such as getting intensity or position data. For example, the user can build the hyperobject using manually methods such as set data(data) and setposition(position) and setlabel(label). The upcoming examples will explain how to use most of the following methods:

Non returning methods

```
# set a Pandas DataFrame as intensity (data)
mapa.set_data(data)
# set a Pandas DataFrame as position (xy)
mapa.set_position(position)
# set a Pandas Series as wavenumber
mapa.set_wavenumber(calibration)
# set the resolution (pixel size )in µm
mapa.set_resolution(res)
# set label name to the pixels
mapa.set_label(label)
```

```
# set sublabel name to the pixels
mapa.set_sublabel(sublabel)
# set name of the hyperobject
mapa.set_name(name)
# append another hyperobject
mapa.append(hyperobject)
# reset index enumeration
mapa.reset_index()
# concatenation of hyperobjects
mapa.concat([hyperobject1, ...])
# remove specific spectrum/pixel at index
mapa.remove_spectrum([index])
# clean data according defined label pixels
mapa.clean_data()
# clean position according defined data pixels
mapa.clean_position()
# clean label according defined data pixels
mapa.clean_label()
# rename labels by two lists (before and after)
mapa.rename_label([before], [after])
# remove specific label name by a list
mapa.remove_label([list])
```

Returning methods

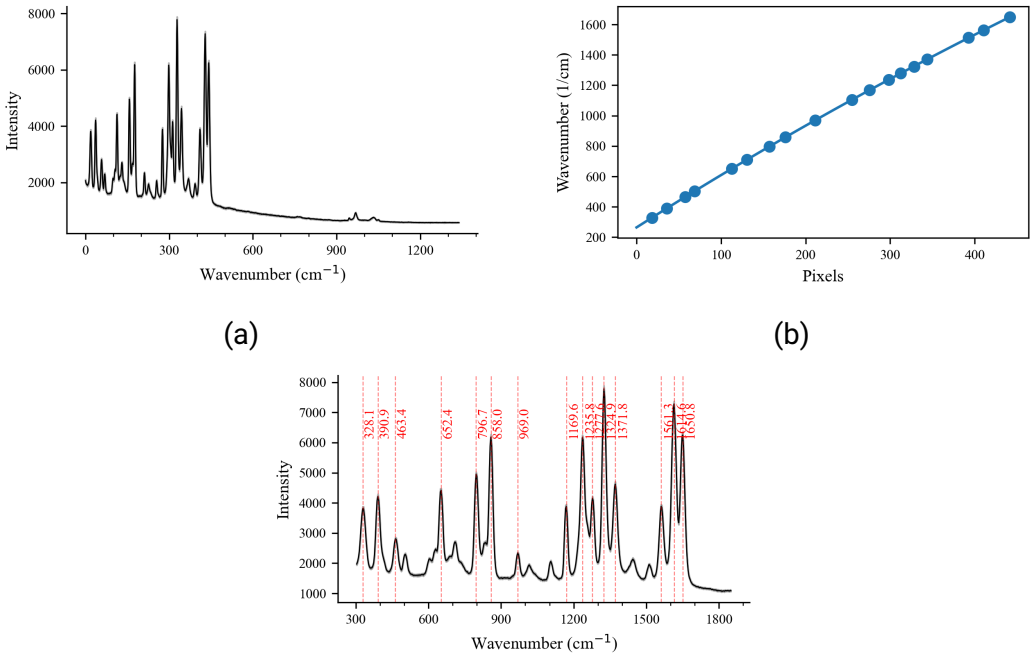
```
#Obtaining intensity
data = mapa.get_data()
#Obtaining positiion
position = mapa.get_position()
#wavenumber
wavenumber = mapa.get_wavenumber()
#copy of the original hyperobject
copied = mapa.copy()
# label
label = mapa.get_label()
# sublabel
label = mapa.get_sublabel()
# name
name = mapa.get_name()
# selection specific label
label = mapa.select_label(list)
# show and get wavenumber positions of the peaks
peaks = mapa.show2(True, prominecence, color)
```

2 Raman Calibration

2.1 Wavenumber calibration

```
from spectramap import spmap as sp # reading spectramap library
### Paracetaminol
mp = sp.hyper_object("para")
#read data with columns in pixels
mp.read_csv_xz("para")

copy = mp.copy() # copy data
# finding peaks of para (next plot)
peaks = copy.calibration_peaks(mp, 0.05)
# determining regression for the calibration
copy.wavenumber_calibration(peaks)
# set the new wavenumber to the original
mp.set_wavenumber(copy.get_wavenumber())
mp.keep(300, 1850)
mp.show2(True, 0.1, "r") # add peaks (not inline mode)
```



(a) (b)

(c)

Figure 2: Wavenumber calibration, (a) paracetamithen spectrum in pixels, (b) calibration and (c) spectrum calibrated

2.2 Intensity calibration

```
# creating reference hyper object
reference_trial = sp.hyper_object("reference")
# reading the lamp referece data along wavelength
reference_trial.read_single_spc("reference")
# showing the spectrum in the next plot
reference_trial.show(True)
# creating hyper object
measured_trial = sp.hyper_object("measured")
# reading lamp experimental data
measured_trial.read_single_spc("lamp")
# keeping finger print region
measured_trial.keep(400, 1900)
# showing the plot as the next figures shows
measured_trial.show(True)

sample = sp.hyper_object("sample")
sample.read_single_spc("sample")
sample.keep(400, 1900) # finger print region
# intensity calibration function
sample.intensity_calibration(reference_trial, measured_trial)
sample.show(True) # showing the calibrated data in the next figure
```

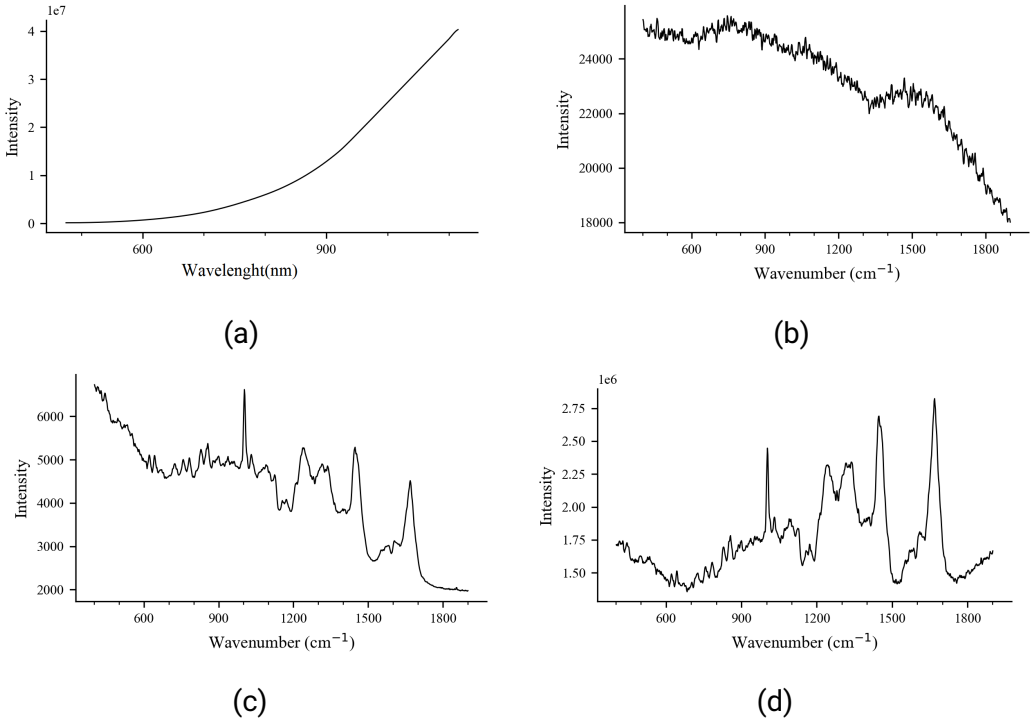


Figure 3: Intensity calibration, (a) reference intensity, (b) measured intensity, (c) uncalibrated sample and (d) calibrated sample.

3 Pre-Processing

3.1 Substraction: background

3.2 Wavenumber intervals

3.3 Filters

3.4 Baseline corrections

3.5 Normalizations

4 Processing

4.1 Unmixing

4.2 Clustering

4.3 Supervised methods

5 Visualization

5.1 Spectra

5.2 Hyperspectral images

5.3 Depth profiling spectra

5.4 3D hyperspectral images

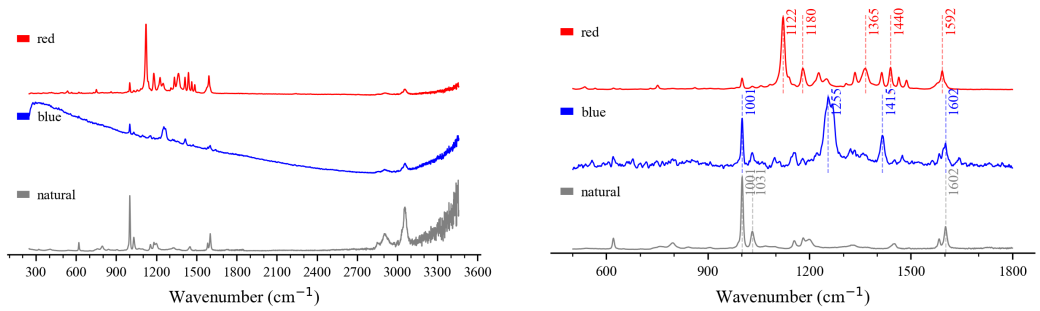
6 Examples

6.1 Plastics

```
from spectramap import spmap as sp
### Defining paths ###
blue_path = 'examples/plastics/blue'
red_path = 'examples/plastics/red'
natural_path = 'examples/plastics/natural'

### Creating and reading the files ###
## Declaring the first hyper object for red sample
```

```
red = sp.hyper_object('red')
## Reading the comma separated vector file
red.read_csv_xz(red_path)
## Setting red name to the whole data set spectra
red.set_label('red')
red.keep(500, 1800) ## Keep finger region
meanred = red.mean() ## Compute mean of all red spectra
## Same procedure for the blue sample
blue = sp.hyper_object('blue')
blue.read_csv_xz(blue_path)
blue.set_label('blue')
blue.keep(500, 1800)
blue.rubber() ## Baseline correction rubber band
meanblue = blue.mean()
## Same procedure for the natural sample
natural = sp.hyper_object('natural')
natural.read_csv_xz(natural_path)
red.set_label('natural')
natural.keep(500, 1800)
meannatural = natural.mean()
### Concataneting the three hyperspectral objects
## create a new empty object
concat = sp.hyper_object('concat')
concat.concat([meanred, meanblue, meannatural])
## show the spectra (see Fig. 5.4)
concat.show_stack(0,0,['red', 'blue', 'gray'])
```

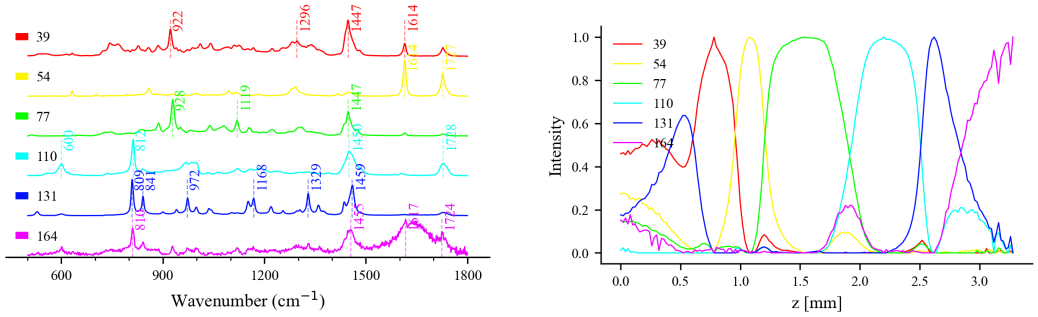


(a) (b)

Figure 4: SpMap processing, (a) Raw and (b) processed data

6.2 Depth profiling of multilayer of plastics

```
from spectramap import spmap as sp
### reading ###
path = 'examples/layers/layers'
stack = sp.hyper_object('layers') #creating the hyper object
stack.read_csv_xz(path) #reading the csv file Wavenumber (cm-1)
### preprocessing ###
stack.keep(500, 1800) #finger print selection
stack.rubber() #baseline correction
stack.vector() #vector normalization
### processing ###
endmember = stack.vca(6) # vertex component analysis
# visualization of spectra and strong peaks(Fig.5.6(a))
endmember.show_stack(0.3, 0, 'auto')
# concentration estimation by NNLS
abundance = stack.abundance(endmember, 'NNLS')
 # set resolution of 20 µm for the profile
abundance.set_resolution(0.02)
# plot profile (Fig.5.6(b))
abundance.show_profile('auto')
```



(a) (b)

Figure 5: Example 2, (a) plastics and (b) depth profile

6.3 Microplastics in tissue

6.4 3D hyperspectral image

```
from spectramap import spmap as sp
import pandas as pd

### reading ###
```

```
path = 'examples/3D/cube'
cube = sp.hyper_object('cube') #creating the hyper object

pre_result = pd.read_table(path+'.csv.xz', sep=',')
#reading the 3d csv file and placing theresolutions xy = 60 µm and z = 70 µm
cube.read_csv_3d_xz(path)
### preprocessing ###
cube.keep(500, 1800) #finger print selection
cube.airpls(100) #advanced baseline correction
cube.vector() #vector normalization
### processing ###
vca = cube.vca(4) # number of expected components
vca.show_stack(0, 0, 'auto')
# concentration estimation by NNLS
abundance = cube.abundance(vca, 'NNLS')
# 3d plot of all clusters (Fig. 5.8(b-c))
aux = abundance.show_intensity_volume(0.5)
```

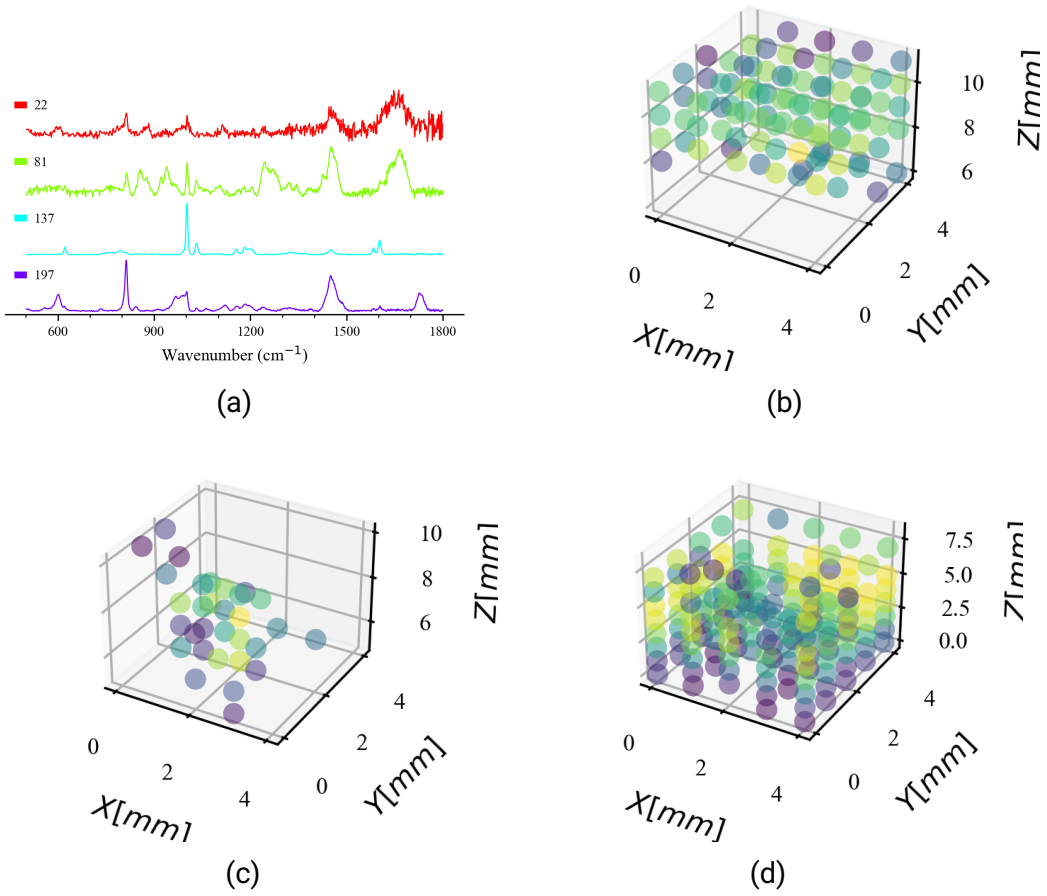


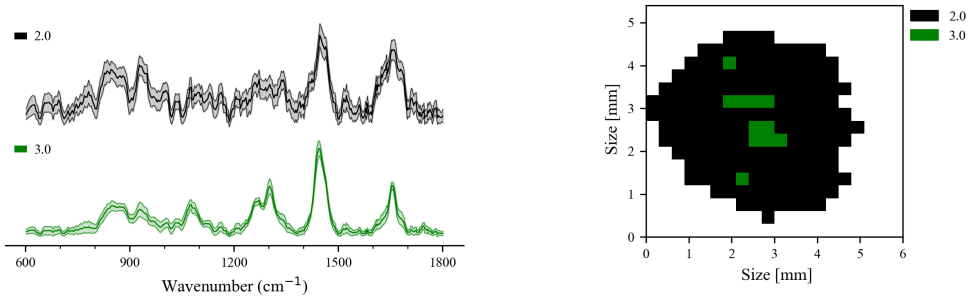
Figure 6: Example 4, (a) VCA results, (b) upper layer (tissue-green color), (c) microplastic (cian) and (d) lower layer (PMMA - purple)

6.5 Infrarred Image

6.6 Bladder

```
from spectramap import spmap as sp
bladder = sp.hyper_object("bladder")
bladder.read_csv_xz("bladder")
bladder.set_resolution(0.3) ## 300 µm step size resolution
bladder.vector() # vector normalization
original = bladder.get_data() ## get data
### K-means clustering
bladder.kmeans(3) #K-means clustering: 3 components
bladder.remove_label([1])
colors = bladder.show_map(['black', 'green'], None, 1) #
```

```
bladder.show_stack(0, 0, colors) #show stack of the clusters (Fig. 5.5(c))
```



(a) (b)

Figure 7: Example 5, (a) spectra of bladder and (b) hyperspectral image.

6.7 Unmixing and clustering of Bladder Hyperspectral Images

```
from spectramap import spmap as sp
#%% reading csv.xz files
bladder = sp.hyper_object("bladder") ## the library
bladder.read_csv_xz("long_bladder")
#%% first sight of the spectra
peaks = bladder.show2(True, 0.2, "r") # basic plotting
#%% processing data
bladder.rubber() # rubber band baseline (basic)
bladder.gol(11, 3, 0) #savitzky golay filter
## remove lipids
bladder.remove_label(['Lipid+Protein', 'Protein+Lipid',
'Tumor+Lipid'])
## remove nonclear data
bladder.rename_label(["Tumor+Fibrosis+Protein", "Necrosis+Tumor",
"Tumor+Necrosis"], ["Tumor", "Necrosis", "Necrosis"])
bladder.rename_label(["Tumor", "Necrosis", "Protein", "Lipid"],
["T", "N", "P", "L"]) # rename labels
bladder.show_spectra(0, 0, 'auto')
## principal component analysis
scores, loadings = bladder.pca(3, False)
## show stacked plot
loadings.show_stack(0.2,1,"auto")
## show scatter plot
scores.show_scatter(bladder.get_label(), 18, "auto")
# hierarchical clustering analysis
bladder.hca("euclidean", "ward", 0.5, 12)
```

```
scores.show_scatter(bladder.get_label(), 18, "auto")
bladder.show_spectra(0,0,"auto")
```

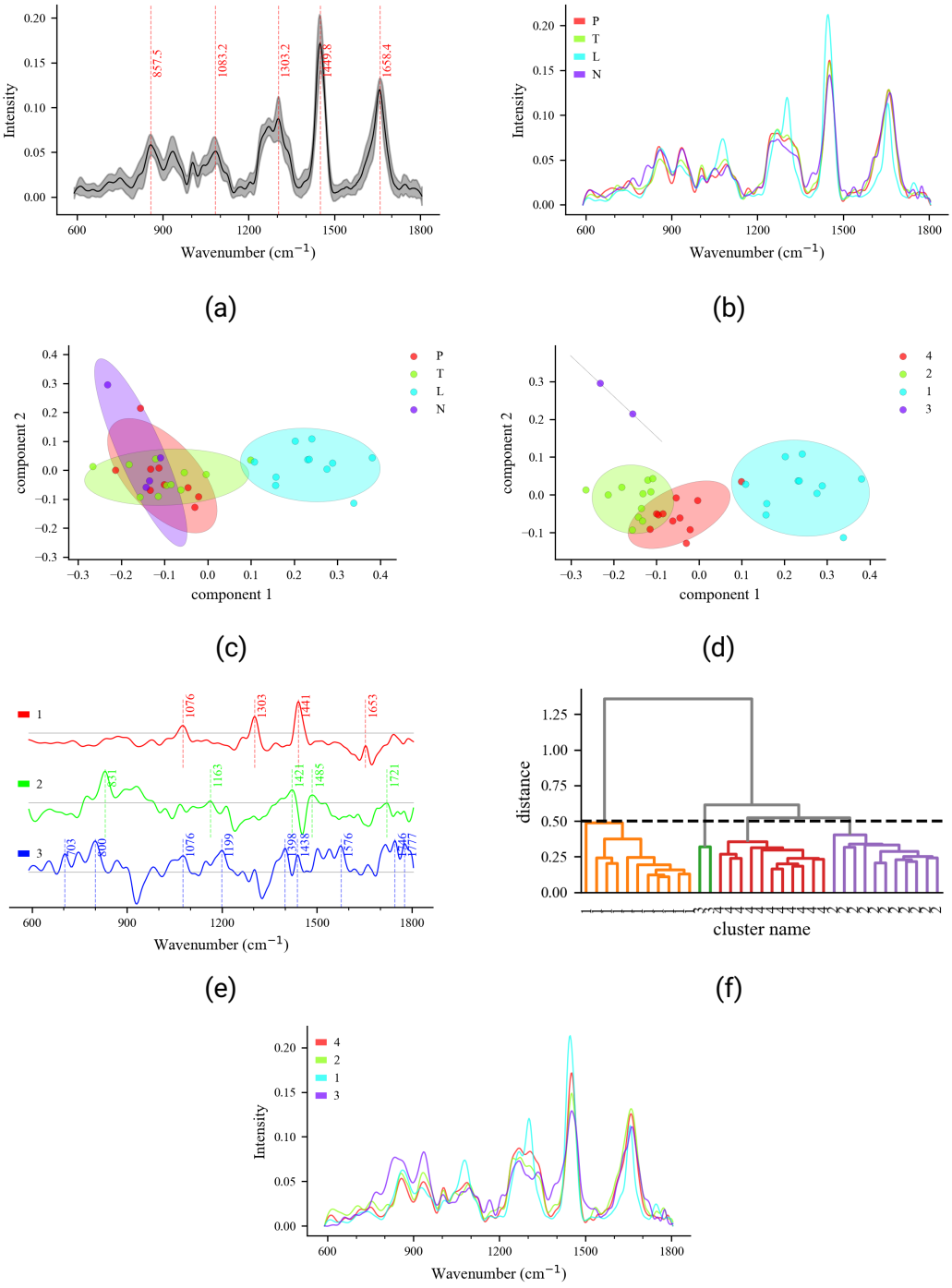


Figure 8: Example 6, (a) raw average, (b) clean data, (c) PCA scatter of scores, (d) PCA scatter using HCA clustering, (e) PCA components, (f) HCA dendogram and (g) cluster components.

6.8 Unmixing PCA and PLS-LDA of plastics

```
from spectramap import spmap as sp
plastics = sp.hyper_object('plastics')
plastics.read_csv_xz('layers')
plastics.show(True)
# keeping finger print region
plastics.keep(400, 1850)
plastics.gaussian(2) # appliying gaussian filter
plastics.rubber() # rubber baseline correction
plastics.vector()
plastics.kmeans(6) # kmeans clustering example for main_label
main_label = plastics.get_label() # saving the main_label
main_label.name = "main_label" # renaming the title of the label
plastics.show_stack(0,0, "auto") # showing the 6 components
# 3 components pca
scores_pca, loadings_pca = plastics.pca(3, False)
# showing scatter with sublabel
scores_pca.show_scatter(main_label, 15, "auto")
# 3 components pls-lda  and 70% training data
scores_pls, loadings_pls = plastics.plslda(3, 1)
# showing scatter with sublevel
scores_pls.show_scatter(main_label, 15, "auto")
```

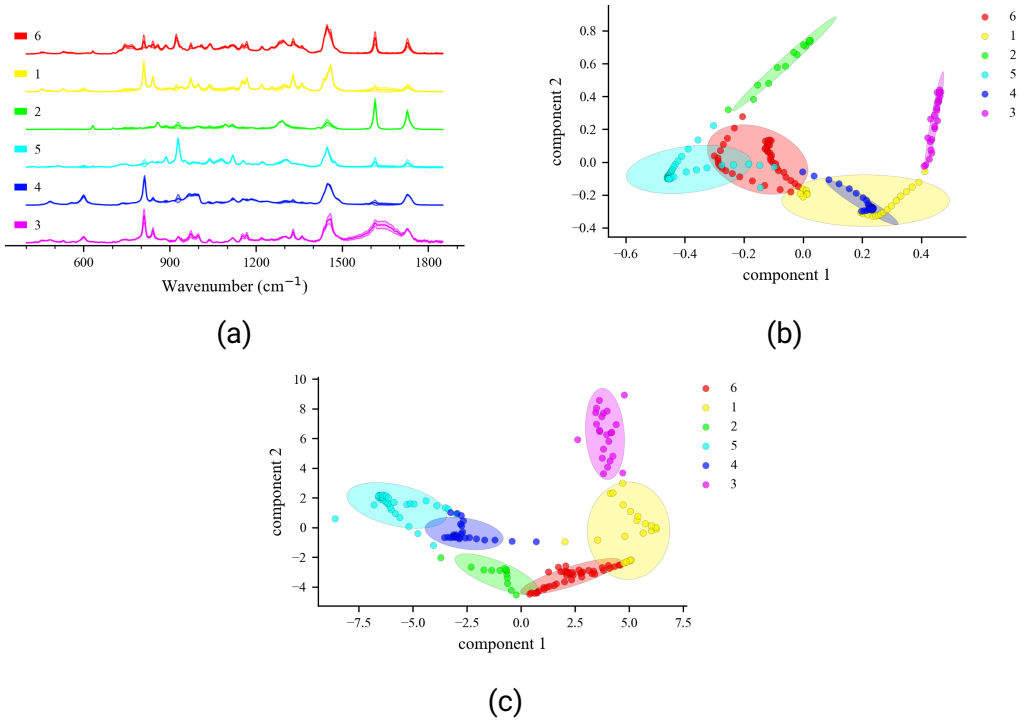


Figure 9: Example 8, (a) plastics, (b) PCA scores and (c) PLSLDA scores

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