Report on the First PortASAP Hackathon (Training Schools) – DIY OSHW for Wine Analysis
11 and 12 of March 2019,
Fábrica Centro Ciência Viva, Aveiro, Portugal.

DISCLAIMER

This report gathers results obtained during the First PortASAP Hackathon (http://portasap.eu/training-school---portasaphackathon-2019.html). It describes instruments that were built and tested during this event and aims, without pretention, to share ideas, tricks or information that may help anyone to make such simple instruments. This report was compiled by G. Erny (PortASAP chair), E. Karamehmedovic (WG Leader) and C. Degrigny (WG Leader) of the PortASAP COST Action (http://portasap.eu/). We are also thankful to P. Kuban, M. Elumalai, A. Pyran for their contribution to this report and all the participants to this event.

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PortASAP
COST Action CA16215 - European Network for the Promotion of PORTable, Affordable and Simple Analytical Platforms

1. Participants

1.1. Organising Committee and Local Organisers

The training school was organised by Guillaume Erny (Action Chair) with the collaboration of all the trainers and trainees. One month before the event, a One Note document was created to organise, plan and share information. Most trainees and trainers participated in the discussion allowing to plan the design, experiments and the needed materials.

Fábrica Centro Ciência Viva de Aveiro hosted the Training School. Fábrica has been open to the public since the 1st of July 2004. It results from a partnership between the University of Aveiro and Ciencia Viva, the Portuguese National Agency for Scientific and Technology Education. Fábrica recently invested in a maker space, called Dóing (Fig. 1), that was used to host the training school. Dóing is equipped with three 3D printers, a 3D scanner, a technical room with laser etching, electrical saw and drill, and more.

Figure 1. The maker space Dóing in Fábrica Centro Ciência Viva de Aveiro

The Training school participants were welcomed by Prof. Pedro Pombo, director of Fábrica. Besides, three employees of Fábrica were present during the two days to help the participants in using the different instruments and provide other necessary assistance.

1.2. Trainers

Apart from the trainers from Fábrica that provided support for the 3D printers and other small instruments, the COST Action supported three other trainers.

- Guillaume Erny (Portugal), the chair of the Action was present to provide technical support in data processing and Matlab programming
- Nuno Ratola (Portugal), the STSM coordinator, was present to provide technical support and sample preparation and Analytical Chemistry (theory and practice)
- Daniele Paesani (Italy, Early Career Investigator (ECI)) was present as an expert in electronics, and DIY instrumentation.

1.3. Trainees

The CORE Group of the COST Action selected the trainees. Participants were asked to send with their application a motivation letter (http://portasap.eu/training-school---portasaphackathon-2019.html). Participants were selected to insure (1) gender balance, (2) geographic diversity and (3) promoting ECI. We received 24 excellent applications for 20 places. In the end, all candidates were accepted, still respecting the budget agreed in the 2nd Grant Agreement and meeting the criteria listed above. An additional candidate joined the training school covering her own expenses (no reimbursement claimed). This trainee submitted her application after the deadline. Table 1 summarised the trainees that were selected.

Table 1. Trainees that participate in the training school

Name	Country	ECI	Group
Antonov, Liudmil	Bulgaria	N	6
Auzins, Krisjanis	Latvia	Y	1
Barkane, Anda	Latvia	Y	3
Boni, MIha	Romania		4
Boumbarova, Neviana	Bulgaria	N	6
Brito, Elsa	Portugal	Y	4
Dinache, Alexandru	Romania	Y	4
Dinache, Andra Cristin	Romania	Y	4
Dodigovic, Filip	Croatia		6
Elumalai, Monisha	Portugal	Y	3
Herceg, Lamija	Bosnia and Herzegovina		2

Kaufman, Daniel	Israel	Y	5
Kleiman, Shani	Israel	Y	5
Kubáň, Petr	Czech Republic	N	5
Laganovska, Katrina	Latvia	Y	1
Larosa, Claudio	Italy		5
Mc Donnell, Kirsty	Ireland		5
Mehmedagic, Dino	Norway		2
Oliveira, Hugo	Portugal		6
Petric, Marko	Croatia		6
Puran, Amina	Bosnia and Herzegovina	Y	2
Sakač, Nikola	Croatia		6
Solomou, Nikolitsa	Greece	Y	3
Zolotarjovs, Aleksejs	Latvia	Y	1
Ćenanović, Mustafa	Bosnia and Herzegovina	Y	2

2. Goals of the Training School in relation to the MoU objectives and objectives of the Grant Period (GP2)

2.1. Goals of the training schools

As defined in the Memorandum of Understanding (MoU), the challenge of this Action is to "Develop and promote low-cost instruments and open-source hardware (OSH) capable of sensitive chemical analysis in specific areas and applications where the use of complex laboratory-based instrumentation is not the desired option". Many approaches could be used, and those should be selected depending on the application and results expected. Nevertheless, a spectroscopic based detection module will often be present. The past decade has been particularly interesting for the development of low cost and Open-source hardware (OSHW) spectrophotometer in the UV-Vis range[1–3], NIR range[4] or Raman[5,6]. Companies, such as Hamamatsu[7], are now selling mini-spectrometer at a reasonable price that can be easily interfaced to Arduino-like platform, smartphone and microfluidic platforms[8]. Price of DIY spectrometers ranges from few thousands of euros to less than 5 euros. The difference of price having mostly to do with the optics involved and the light sensor.

Interestingly, the camera of a smartphone is a very potent light sensor in the visible range and many low-cost solutions are now designed to incorporate a smartphone, not only for sensing but also for data analysis, software and data transfer[9–12]. In spectrometry, the American citizen group, Public Lab, designs and promotes foldable spectrometer for smartphone[13], desktop[14], or even made from Lego blocks[15]. While such simple designs are invaluable tools for teaching spectrometry and democratising science[16], essential questions related to reliability, repeatability and reproducibility remain open.

Thus, the main goal of this training school was to test foldable spectrometers for the analysis of wine. While wines are very complex samples that are usually analysed using large instruments (LC or GC-MS, NMR) or infrared and- near-infrared spectroscopy[17], it has also been demonstrated that UV-VIS spectroscopy with chemometrics analysis, can be used to classify wines [18–20]. The Aveiro training school/Hackathon on wine analysis aimed to gather 25 scientists from different fields and allow them, by group, to build freely foldable spectrometers. Instruments were used to analyse the same set of wines samples with varying factors of dilution. Results were then analysed to determine whether clustering patterns emerged independently of the instruments and smartphone used. The results were supposed to indicate the applicability of the low-cost spectrometer in some aspect of wine analysis.

2.2. Goals of the training school in relation to the goal of the MoU and GP2

This training school fulfilled the following MoU objectives

- **Challenge:** Develop and promote low-cost instruments and open-source hardware (OSH) capable of sensitive chemical analysis in specific areas and applications where the use of complex laboratory-based instrumentation is not the desired option.
- **Research Coordination 1:** To coordinate intersectoral, international and interdisciplinary studies in complex environments to test and validate OSH tools. This objective will involve citizen science initiatives (i.e. water quality in the Venetian Lagoon and Irish loughs).
- **Research Coordination 2:** To provide detailed reports on existing open-source hardware and their field of application and assess their limitations. this will be done by maintaining a database of open-source hardware, to present and demonstrate their fabrication (video tutorials) and to validate each instrument with interlaboratory studies.
- **Capacity Building 2:** To encourage research facilities and SMEs to use open-source hardware.
- **Capacity Building 4:** To attract and facilitate the mobility and the multidisciplinary training among the different protagonists of the Action, during which attention will be drawn to maximise the benefits for all participants.

The training school also fulfilled the following objective of the Grant Period (GP2: 01/05/2018 – 30/04/2019)

- **#1:** Development of simple OSH analytical platforms for workshop/training school.
- **#3:** Create an open repository of experimental data from members of this COST Action
- **#8:** To organise and promote short-term scientific missions to improve the exchange of knowledge, promote long-term collaboration, build synergies and participate in the formation of a new generation of researchers
- **#11:** To promote Open Source Hardware as a reliable alternative to classical instruments

3. Activities

The first day of the training school was devoted to the fabrication of the spectrometer while the second day focussed on its testing, calibration and analysis of samples. Trainees were divided in groups of three to six people; the formation of the groups are summarised in Table 1.

3.1. General design

3.1.1. Group #1 - Auzins, K.; Laganovska, K.; Zolotarjovs, A.

<u>Microspectrometer based on Hamamatsu C12880MA</u>

This group brought the instrument that is being developed at their institution. It is based on the Hamamatsu C12880MA chip and is run via an Android application and connected by Bluetooth. The spectrometer covers a range from 350nm to 750nm.

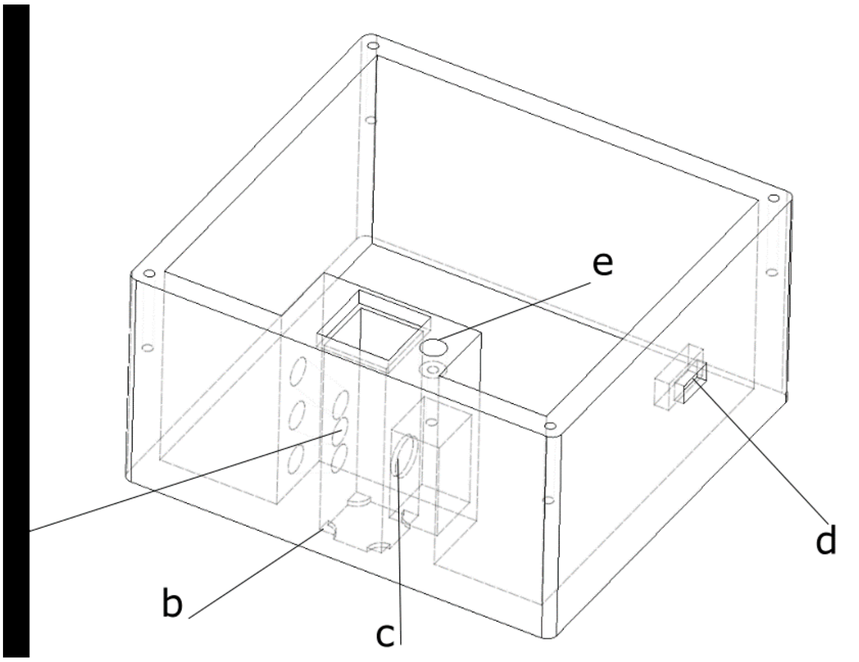


Figure 2. Overview of the main body. a – mounting spots for LEDs, b – stop features for the cuvette, c – opening and mounting point for C12880MA unit, d – on/off switch mounting point, e – fixing screw hole for C12880MA unit.

During the workshop, the group designed and tested an adjustable input slit width holder. The holder was designed to be used with razor blades as flaps (Figure 3). There would be a 3mm screw-on top that pushes on the wedge which would push the blades outwards. The groove around the perimeter is meant for rubber band which would apply inward pressure on the razor blades, thus preventing them from moving.

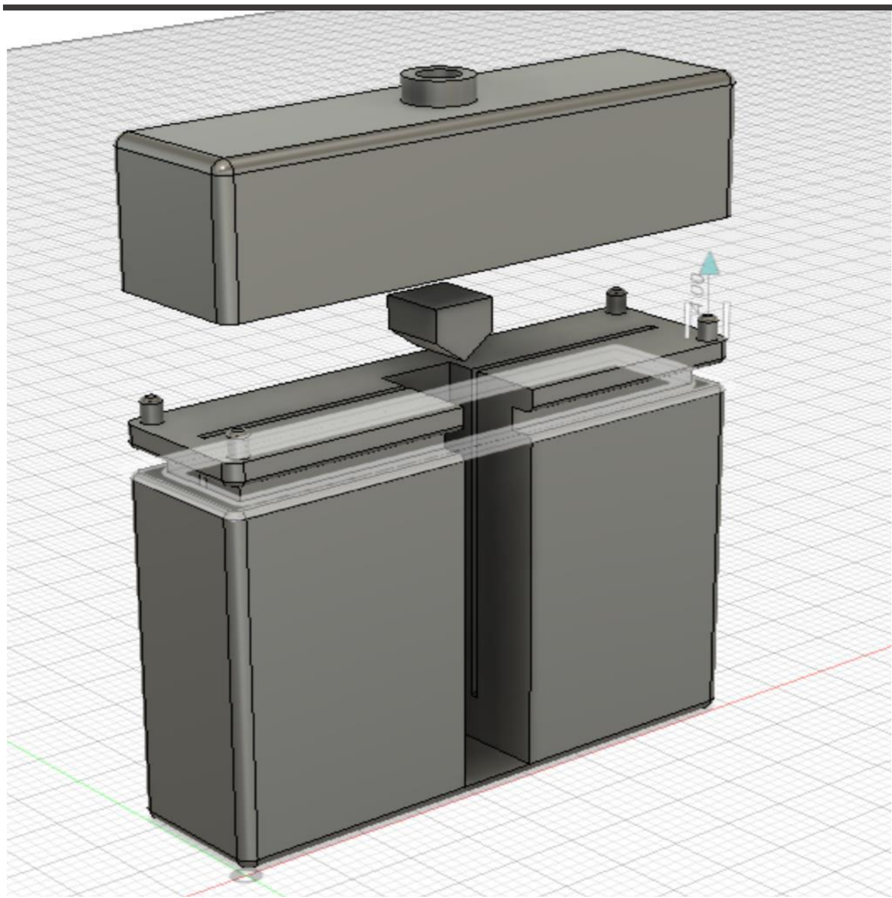


Figure 3. Adjustable input slit width holder

3.1.2. Group #2 - Ćenanović , M.; Herceg, L.; Mehmedagić, M.; Puran, A.,

Many may find this project challenging since all components are very sensitive and require precise and accurate measurements and calculations. Further, it has a complex structure and all parts are in some way related. This means that change in one variable in input can make a huge difference at the result at output. One of the most important is in Chemistry, in Liquid analysis. At this hackathon, we used it in liquid analysis.

The spectrophotometer was constructed according to the paper template from https://publiclab.org/notes/warren/11-30-2017/build-a-papercraft-spectrometer-for-your-phone-version-2-0. A picture of the built spectrometer is found in Figure 4.

Figure 4. Instrument built by Group 2

3.1.3. Group #3 – Anda, B.; Monisha, E.; Nikolitsa, S.

Description of the spectrophotometer:

The spectrophotometer was constructed according to the paper template from https://publiclab.org/notes/warren/11-30-2017/build-a-papercraft-spectrometer-for-your-phone-version-2-0.There were some modifications to the design. The template was cut from a black paper and a cover was added where removable cuvette goes in, to ensure that no extra light is disturbing the measurement. For grating, a stripped DVD-R (Verbatim) was used as per instructions. With the help of ethanol, we were able to remove the azo dye. Slit part of the construction was replaced with the razor blade at first, but later it was discovered that by adding black tape directly on the cuvette gives more precise measurements. A paper cuvette holder was made that had two holes thus made the use of the portable spectrometer way easier. The light source was an LED lamp that contained about ten cool white LEDs, one in the middle.

Various types of wines were tested from highly dark red wines to rose by transferring each sample to a cuvette then ready to be tested in our portable spectrometer. The process was quite easy. The light was shed through the slit to our sample and with the help of the front camera of a Samsung Galaxy A8 we were able to take pictures of the dispersion colour stripes (as seen in Figure 5 below). As known, the slit determines the amount of light (photon flux) that enters the optical bench and it is probably the most important part of a spectrometer. In our case, the width of the slit was proven satisfactory as the performance of our spectrometer was good. The pictures taken with the front camera were sent to a data processing module created with Matlab that was able to give us the spectrum curve according to each and every one of the colour stripes images.

In that way the front camera was used as the detector of our portable spectrometer.

Figure 5. Photo of a setup and required supply materials

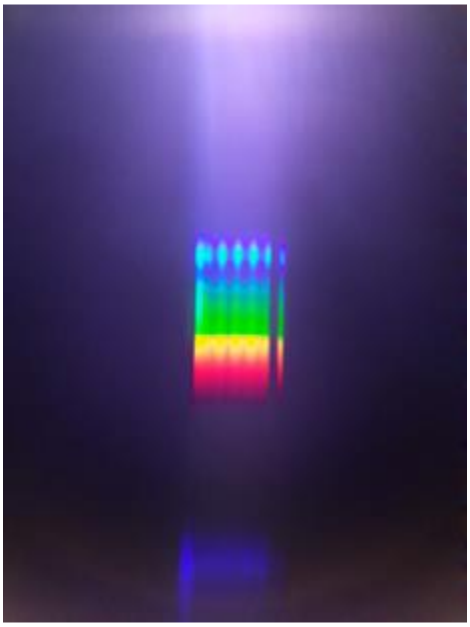
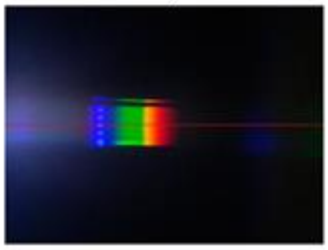


Figure 6: Photo of the front camera of a Samsung Galaxy A8 of the colour stripes to be used for spectral analysis

Note from the team:

Important refraction was observed, and as it can be seen bellow (Figure 7) most of the spectra were heavily saturated. Information below 1500 pixels lost.



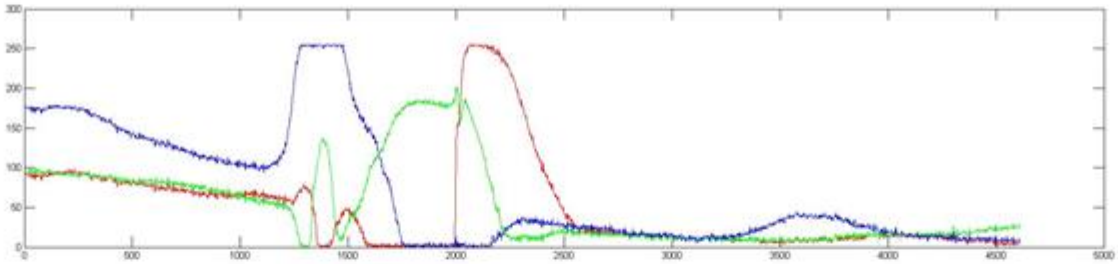


Figure 7. Photo and corresponding spectra obtained from a wine sample.

This issue can be solved in the future by increasing the wine concentrations, using filters or changing the light source. Nevertheless, significant differences were observed between samples.

Due to the light saturation, these results were not used for the final comparison.

3.1.4. Group #4 –

No description was provided by this group

3.1.5. Group #5 - Kubáň, P.; Kaufman, D; Kleiman, S.; Larosa, C; Mc Donnell, K.

Description of the spectrophotometer:

The spectrophotometer was constructed according to the paper template from https://publiclab.org/notes/warren/11-30-2017/build-a-papercraft-spectrometer-for-your-phone-version-2-0

There were some modifications to the published design. The template was cut from a black paper. For grating, a stripped DVD-R (Verbatim) was used as per instructions. The azo-dye from the DVD-R was removed with ethanol. The slit part of the spectrophotometer was printed on a 3D printer and was 1.5 mm wide. The slit was glued with the tape to the spectrophotometer tube instead of using the paper template. A paper cuvette holder was made that had two holes; the incoming light hole was about 2x1 mm (WxH), the hole that was placed on the slit was about 10x1 mm (WxH). The light source was a LED lamp that contained about ten cool white LEDs, one in the middle. A black shield with a 5 mm hole was placed on the LED lamp to shield the light from all but one LEDs. Also, a sheet of white paper was placed in front of the LED lamp to decrease the intensity of the light. The LED was glued with tape as close as possible to the cuvette hole (2x1).

Figure 8. Setup photo

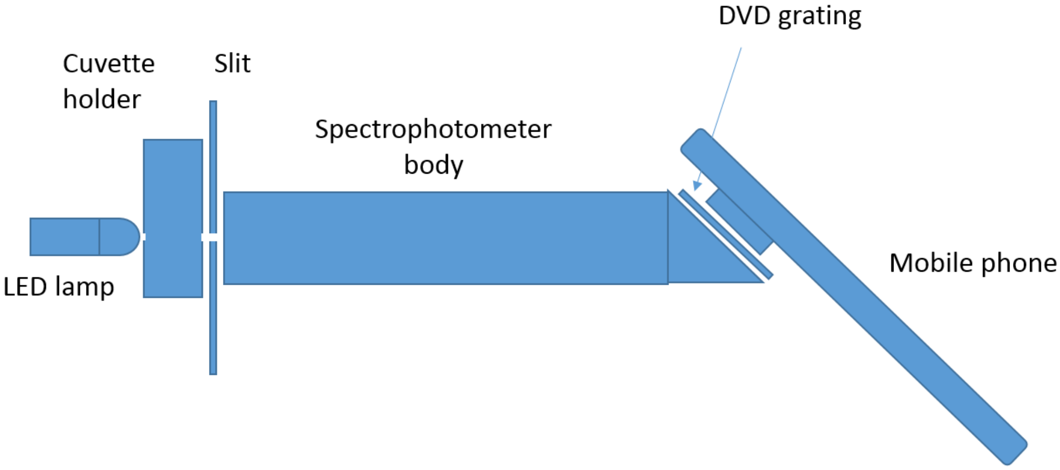


Figure 9. Setup schematic

3.1.6. Group #6 -

No description was provided by this group

3.2. Samples list

For the training schools, trainees were asked to bring a bottle of red wine from their country. The list of the wines, with some information when available, are summarised in Table 3.

Table 3. List of wines used for the training school.

#	Name	Country	Type	Year
1	Campo Viejo	Spain	Red – Tempranillo; Graciano; Meruelo	
2	Monte Velho	Portugal	Red – Aragonez; Trincadeira; Touriga National; Syrah	2017
3	Barkan	Israel	Red – Cabernet Sauvignon	2015
4	Nemea	Greece	Red - agiorgitiko	2017
5	Laroso	Italy	White – home production	2018
6	Só Pias	Portugal	Red	NaN
7	Dealumare Rose	Romania	Rose	2018
8	Porca de Murça	Portugal	Red	2017
9	Dealumare Feteascã Neagrã	Romania	Red - Feteascã Neagrã	2017
10	Dealumare Cabernet Sauvignon	Romania	Red - Cabernet Sauvignon	2017
11	Villa Terres	Bulgarian	Red – Cabernet Sauvignon	2014
12	Alabastro	Portugal	Red – Aragonez; Trincadeira; Alicante Boushet	2016
13	Mediterano Plavac	Croatia	Red	2013
14	Chateau des Jacques	France	Red – Morgon	2014
15	Abavas	Latvia	Black current wine	

4. Results

4.1. Analysis of the resulting data

After passing through the sample, and the spectrometer body (Figure 5) the light is split by the grating film, and the resulting spectrum is recorded as an image by the smartphone. Such images can be opened by numerical-analysis software (R, Matlab or Python (*matplotlib*) for example). The original image is then transformed in 3-dimensional matrices where the intensity of the light for each pixel and each filter is recorded. Analyses were made using Matlab and the following step were performed

- Opening of the image
- Flattening of the 3D image matrix to a 2D matrix by merging the R, G and B matrix, using the highest intensities.
- Smoothing of the 2D matrix using a Savitzky-Golay filter
- Flattening of the 2D matrix to a 1D spectra by recording the max intensity at every column
- Baseline correction

The results of the analysis can be visualised in the figure bellow

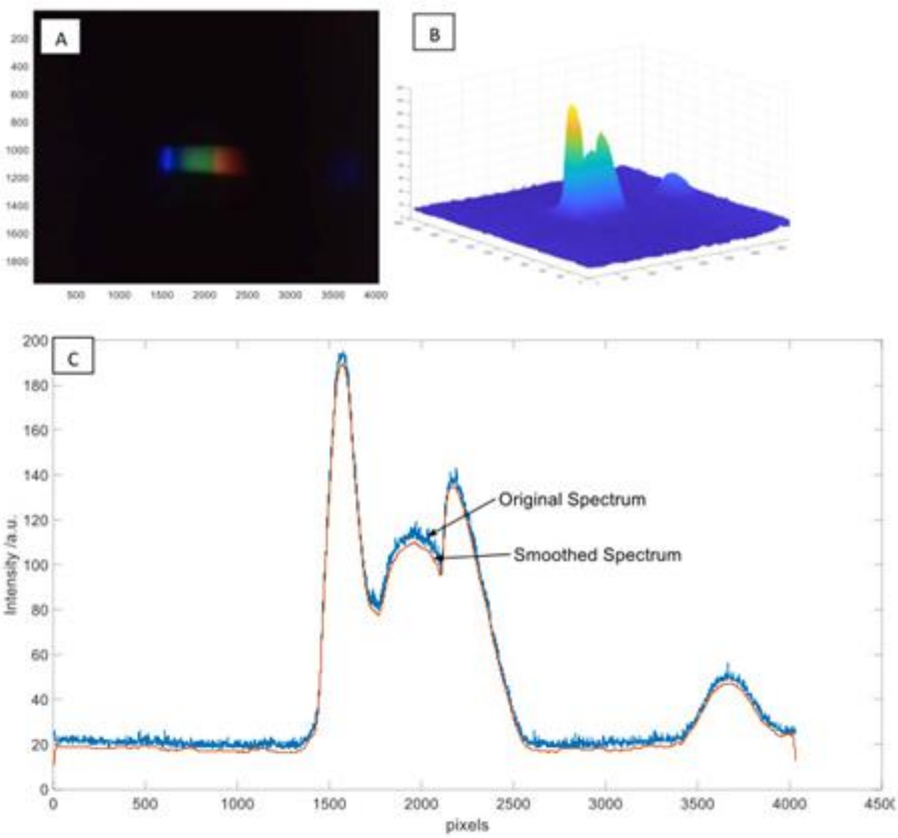


Figure 10. A. Original image, B 2D matrix of data, C. original and filtered spectrum.

4.2. Normalisation

While in most designs, the spectrophotometer was taped to the smartphone body to decrease movement, as it can be seen in Fig 11A, variations along the x-axis are still significant. Change along the x-axis between successive spectra was strived to be minimised and corrected in software. Briefly, the first recorded spectrum was selected as the etalon; variations in the x-axis in subsequent spectra were assumed to follow equation 1.

$$\mathbf{Xc} = a(\mathbf{X} + b) \quad (1)$$

X and **Xc** are the original and corrected x-axis, respectively, *a* and *b* are the fitting coefficients to be determined. Fitting coefficient using the simplex search method and minimising the sum square error (SSE); this was done using the function *fminsearch* in Matlab. Normalised spectra can be seen in Figure 11B.

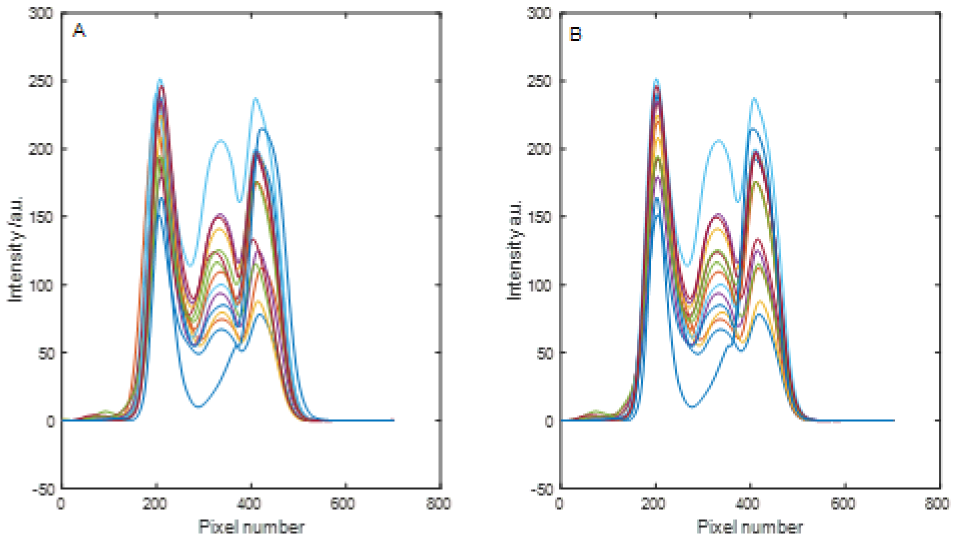


Figure 11. Original spectra obtained with all the sample with a given instrument, B normalised spectra.

4.3. Results

Only results from two groups could be used for comparison; the other ones were either incomplete or saturated. Figure 12 compares the spectra obtained by Group 2 and Group 5.

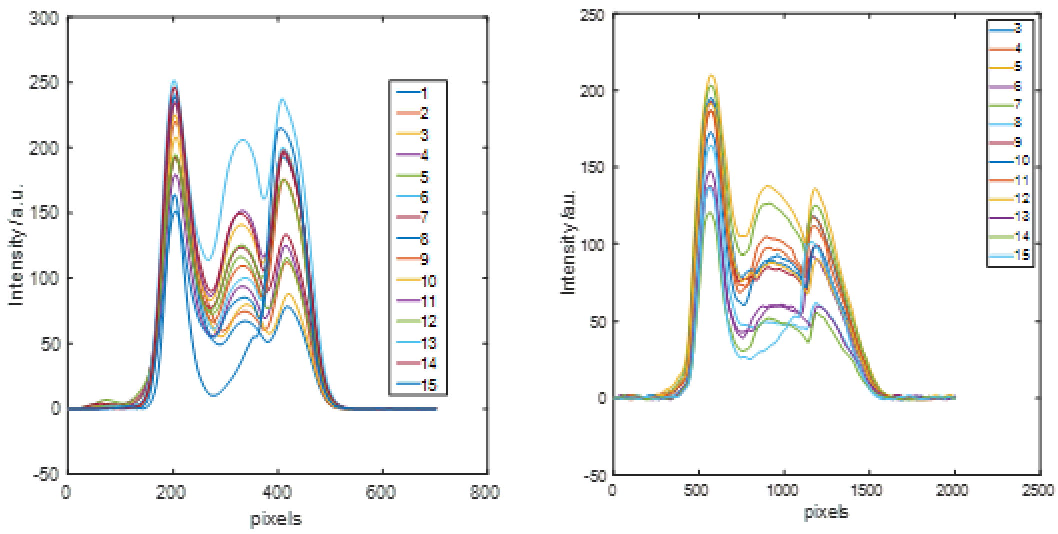


Figure 12. Comparison of wine spectra recorded using the instrument built by group 2(left) and group 5 (right).

Significant differences can be observed between different wine samples in both spectrometers, hinting that such instruments may be suitable for wine fingerprinting. To further explore this, principal component analysis was used, with the goal in comparing the obtained classification. Results are presented in Figure 13.

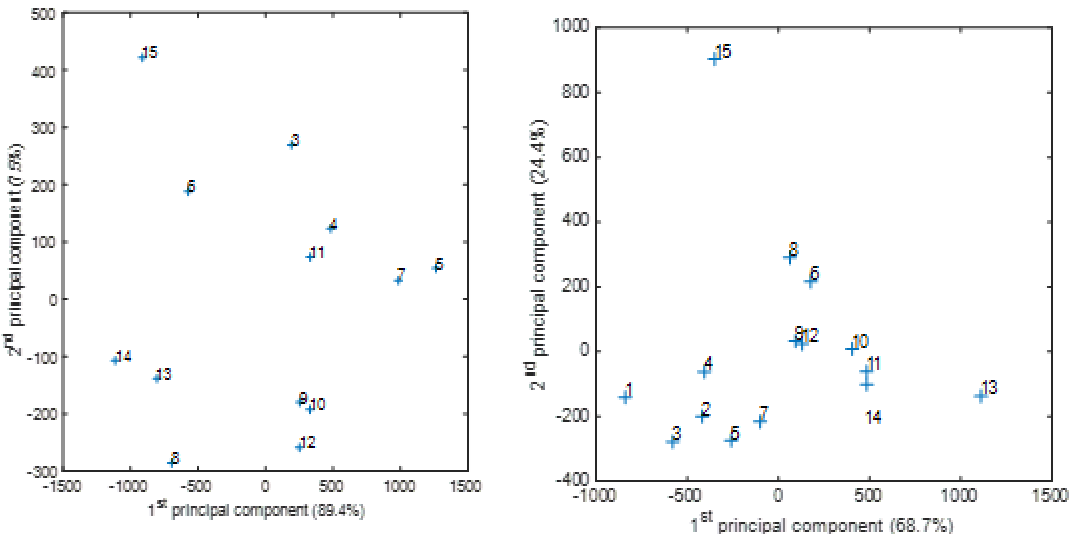


Figure 13. Comparison of PCA of wine spectra recorded using the instrument built by group 2(left) and group 5 (right).

However, in the exception of sample 15 (Black current wine), no clear correlations could be found. This was further investigated using different normalisation (sum of intensities and intensities at peak apex), but no better results were obtained. This is probably due to the absence of standardisation (wavelength and intensity). Nevertheless, results obtained during those two days, designing this very simple OSHW were highly beneficial, and this preliminary work is planned to be continued.

5. References

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