Has the time come to use near-infrared spectroscopy in your science classroom?

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Abstract Smartphones, coupled with small mobile sensors, make it possible to work with near-infrared (NIR) spectroscopy in science classrooms. NIR spectroscopy has become a standard analytical technology in various industries. These new devices enable students to create their own data in real time. This article presents an inquiry-based teaching unit, in which students analyse seemingly identical white crystals in order to find a hazardous chemical substance in the school lab. Using student safety sheets, they develop a risk assessment for themselves and the teacher.

Until recently, when encountering an unlabelled substance in the chemistry lab, one had to dispose of it because it was impossible to identify the substance, given most chemicals are either white crystals or colourless liquids. Moreover, it could not be discarded as general waste since there was no way of knowing whether it was hazardous (ASE, 2018: Topic 11).

With recent developments in miniaturising sensors and in advanced data processing, near-infrared (NIR) spectroscopy has become a standard analytical technology. It is widely used in medicine, agriculture and other industries and research areas, because it delivers real-time results, is non-invasive and sample preparation is often not necessary. The downside is that the method uses 'chemometric models' to interpret data. Hence, any spectrum measured needs to be compared to known substances. Unlike infrared spectroscopy, it cannot directly identify, for example, functional groups. Another limiting factor is that the devices that are potentially affordable for school projects currently only measure a limited range of the spectrum, so it is only possible to distinguish a limited number of molecules. The device used by the students in this article is called SCiO (Figure 1). It works with a consumer-friendly app for mobile phones, which has pre-installed applets to analyse aspects such as nutrient information of food items or body fat. Additionally, it allows students to create their own spectra to compare different substances (SCiO, 2016).

In this article, I present an example of how the device can be used in a student health and safety context, in which students analyse different kinds of chemicals after developing a risk assessment for themselves and the teacher. In order to make the inquiry-based teaching unit more interesting, it is designed as a 'case' that the students have to solve.

This article is based on a presentation at the ASE Annual Conference at Birmingham in January 2019.

Figure 1 Using a mobile near-infrared spectrometer in the classroom

The case – a teaching sequence with a story

A good case tells a story, is relevant to the audience, is conflict-provoking and decision-forcing and should be short (Herreid, 1997). Last but not least, it must have pedagogic utility; only then can we expect to achieve a student-centred approach to learning, which can contribute to critical thinking and lifelong learning skills (Carder, Willingham and Bibb, 2001). Our story to set the scene is very simple.

The students knew in advance that their teacher wanted to surprise them with a little chemistry show. The chemistry lesson starts with the teacher reporting an incident that happened while preparing the evening before. A 'wipe-clean' marker had been used by mistake when preparing a class set of chemicals, and some labels had become unclear after the containers were handled. Some dishes had accidentally slid off a tray onto the bench, causing a little dust in the air, and the teacher felt a distinct irritation in his airways and eyes (Figure 2). He recovered after a few hours, but it was a frightening experience.

The students were challenged to help the teacher make better risk assessments and to examine the unknown substances, with the assignment shown in Figure 3. In order to fulfil the first task, the students need to examine the CLEAPSS *Student Safety Sheets* (CLEAPSS, 2019a) and prepare a risk assessment. We use this case with secondary school students (ages 13–16) but it could easily be adapted for older students.

The question remains: how do we want to let the students analyse the substances?

White crystals, substance analysis and new mobile gadgets

In teaching contexts, students often expect that they will encounter relatively low-hazard substances such as sugar, salt, maybe citric acid or similar 'everyday' household substances. In real life outside the classroom, this isn't necessarily the case. We therefore wanted to unsettle the students a little: is this only a teacher trick or is it actually something hazardous?

Most solid chemicals are colourless (looking white) and odourless crystals, so students and teachers cannot see or smell whether a substance is hazardous. Professional substance analysis includes '*ultra-violet (UV), infra-red (IR) and nuclear magnetic resonance spectroscopy (NMR) or mass spectrometry (MS) … These techniques require specialist knowledge to perform and interpret their output*' (ECHA, 2019).

This means, until now, as a teacher you could not use spectroscopy outside the visible range in your classroom, with hands-on activities for all students. Most of the resources available for teaching are therefore based on animations. Alternatively, if teachers wanted to include hands-on activities in case-based teaching, they would rely on 'traditional' chemical testing, as for example Extance and Turner (2017). The development of ever-smaller and cheaper mobile devices, however, is now resulting in promising hand-held NIR spectrometers (Beć and Huck, 2019; Extance, 2018).

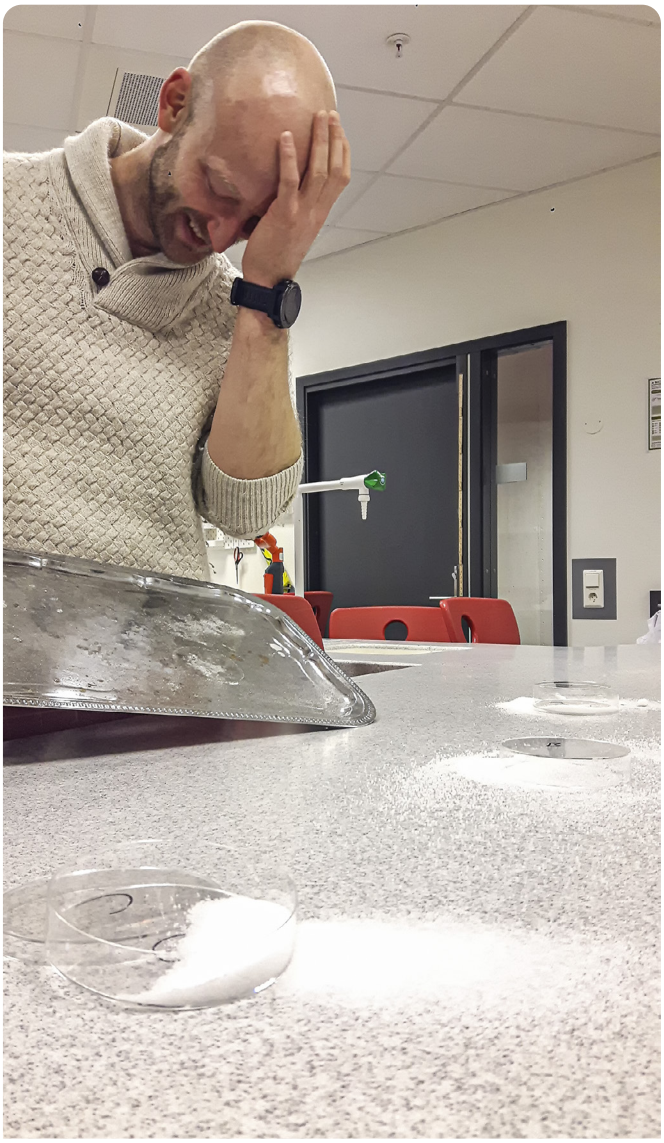

Figure 2 The 'accident' in the lab, which raised health and safety questions

Help me, chemical detectives!

1. **Conduct a risk assessment with your group, using CLEAPSS *Student Safety Sheets* of all eight substances in the lab.**
2. **Discuss your risk assessment with me, before entering the lab.**
3. **Are you able to determine the substance that caused my illness? Use your spectrometers; and remember to document your investigation.**
4. **Prepare a short presentation to discuss and defend your findings with your classmates.**

Figure 3 The students' assignment

How does NIR spectroscopy work?

Substances absorb energy of different wavelengths. The visible part of the electromagnetic spectrum ranges between approximately 400 and 700 nm, and we see those wavelengths as different colours.

The invisible radiation in the infrared wavelengths, above about 700 nm, interacts with atoms and molecules and contributes to the stretching and bending of covalent bonds. Mid-infrared wavelengths, above 2500 nm, can be used to determine distinct groups in molecules, for instance hydrogen-oxygen-bonds of an alcohol (Chemguide, 2019).

NIR spectroscopy is based on the absorption of electromagnetic radiation at wavelengths in the range 780 nm to 2500 nm, measuring, for example, the diffuse reflectance. At the molecular level, an NIR spectrometer measures overtones and combination tones of the molecular vibrations involving covalent bonds with hydrogen (e.g. C–H, O–H and N–H).

The device we used (Figure 4) is coupled to a smartphone app, which sends the data obtained to a server, where it is processed and sent back to the phone. The results are shown as a spectrum (Figure 5).

Unfortunately, the consumer app does not label the two axes quantitatively. This is a pity for science teachers who would like to teach the skill of reading scientific illustrations. When accessing the developer's resources, one finds out that the SCiO sensor covers a short part of the NIR spectrum, approximately 700–1100 nm (Extance, 2018). For a more detailed description of NIR spectroscopy and how to calculate and compare these spectra to known substances, see, for example, Beć and Huck (2019).

Figure 4 The mobile NIR spectrometer. The yellow field to the left is the light source. The incoming radiation is then partly absorbed in the probe and scattered. Only a fraction of the reflected light reaches the sensor to the right and the rest is absorbed or lost.

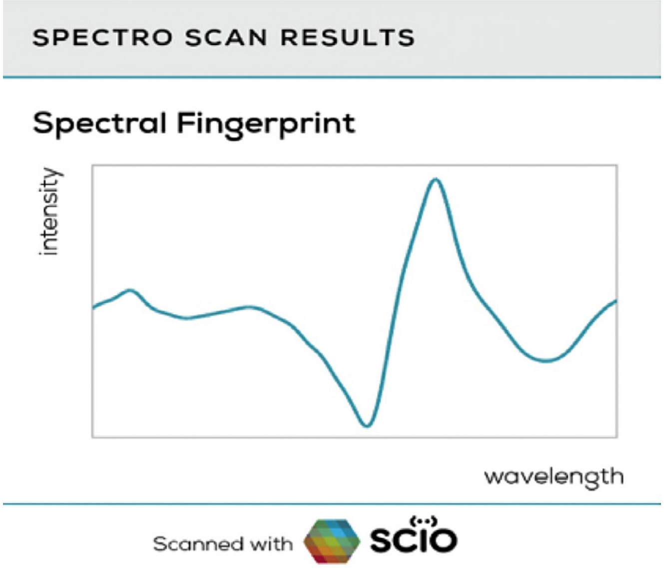

Figure 5 Screenshot from the SCiO Pocket Molecular Sensor app (www.consumerphysics.com); the diagram shows the spectral fingerprint of sucrose, measured by the author

Learning objectives

Our learning objectives for the teaching unit presented in this article are as follows:

1 near-infrared spectroscopy as a method to identify materials and chemicals;
2 health and safety education: risk assessment;
3 arguing and communicating findings.

The science curriculum context for the first objective, in which teachers are able to use the device as more than a black box and can foster critical thinking about the method, aligns with key stage 3 (age 11) upwards (DfE, 2015):

- *use appropriate techniques, apparatus, and materials during fieldwork and laboratory work, paying attention to health and safety;*
- *(chemistry) the identification of pure substances;*
- *(physics) the transmission of light through materials: absorption, diffuse scattering and specular reflection at a surface.*

The second objective aligns with ASE (2018: Topic 2), recommending that:

> *the health & safety principles which students should learn include the following:*
> - *how to recognize and identify hazards;*
> - *how to identify the possible risks from those hazards;*
> - *what actions are needed to reduce those risks to an acceptable level.*

The third objective about 'nature of science' is outside the scope of this article. It is included in the case description below, but for a detailed discussion see, for example, McComas (2017).

The teaching sequence: how to solve the case and make a risk assessment

1. Introducing the spectrometer

The students have to become acquainted with using and handling the mobile device before they can use it to investigate the unknown substances. A quick-start guide is included when buying the devices. Alternatively, videos can be used (SCiO, 2016), or a step-by-step guide for younger students can be requested from the author. I suggest introducing handling, and possibilities and limitations of the device, in another science context beforehand, for instance the investigation of the students' lunch packs. This helps focus them on the topic.

2. Developing a risk assessment

> *To understand hazards and risks in school science, the students must also be taught some science. Without this, they will only ever be following instructions, which they could not apply to future, similar situations, whether in school or outside.* (ASE, 2018: Topic 2)

The students have to learn what a risk assessment is about and how it is performed, according to CLEAPSS (2019a). Once the students leave school, there will not be a teacher providing a 'just-in-time' service, and workplace colleagues or flatmates might not have the required knowledge.

The students are provided with the CLEAPSS *Student Safety Sheets* for each of the eight substances currently in the lab; they will discuss them and fill out the student form for assessing risks (CLEAPSS, 2019a), before reporting back to the teacher.

Before being allowed to enter the lab and analyse the chemicals, the students have to discuss their risk assessment with the teacher and give advice for appropriate protection measures. In our case, which includes potassium chlorate, these should include eye-protection, lab-coat and gloves.

3. Investigating the substances with SCiO and communicating the results

The students have three options to examine the unknown chemicals:

- take spectro scans and compare them manually;
- build an applet based on the known substances and let the SCiO compare them (Figure 6);
- build an applet based on the unknown substances and let the SCiO compare them.

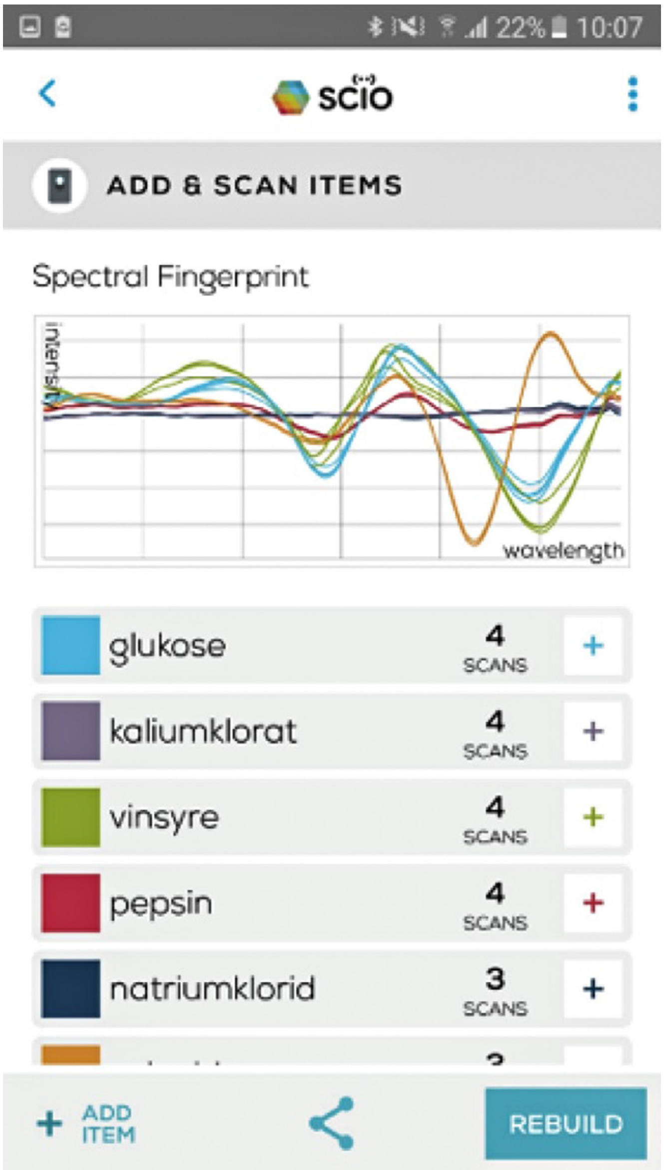

Figure 6 Screenshot from the SCiO Pocket Molecular Sensor app: different organic substances show distinct fingerprints, while NaCl, for example, does not absorb in this part of the spectrum

Whichever approach is used, coordinating and documenting is crucial! This fosters effective group work, as the students are responsible for giving a documented presentation in the end.

Similar cases may be constructed with a variety of 'accidents' and three possible cases are presented below. The students are presented with between one and three unknown substances from a selection of eight substances that are all white crystals and look very similar.

An easy investigation

Present only one substance to the students, for instance sucrose.

Sucrose shows strong and distinct absorbance in the part of the spectrum measured by the spectrometer (Figure 5). It is therefore easy to identify the absorbance spectrum and this is a good choice for younger students. At the same time, sugar has the advantage of not being harmful (from a chemist's point of view). All students and all spectrometers in our test groups managed to identify sucrose with ease.

A more ambitious task

Identify two unknown substances such as sucrose and citric acid (Figure 7). The absorbance spectrum of citric acid looks similar to that of sucrose, so only when comparing the spectra directly will the students notice that the respective peaks are at different wavelengths. Although citric acid is a normal household substance, known to the students as an ingredient of some sweets, it is actually hazardous as a pure ingredient. The CLEAPSS *Student Safety Sheet* lists nearly all the symptoms of illness the teacher reported to the children.

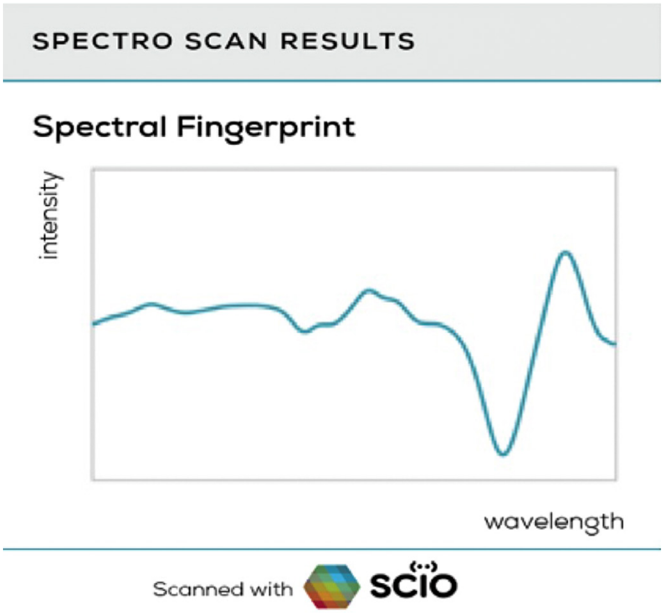

Figure 7 Screenshot from the SCiO Pocket Molecular Sensor app: the diagram shows the spectral fingerprint of citric acid, measured by the author

The tricky one!

Presenting three unknown substances to the students, potassium chlorate V (KClO3), sucrose and citric acid, we are really testing the SCiOs and challenging the students. Potassium chlorate shows no absorption, only a nearly straight line (Figure 8), and, depending on how

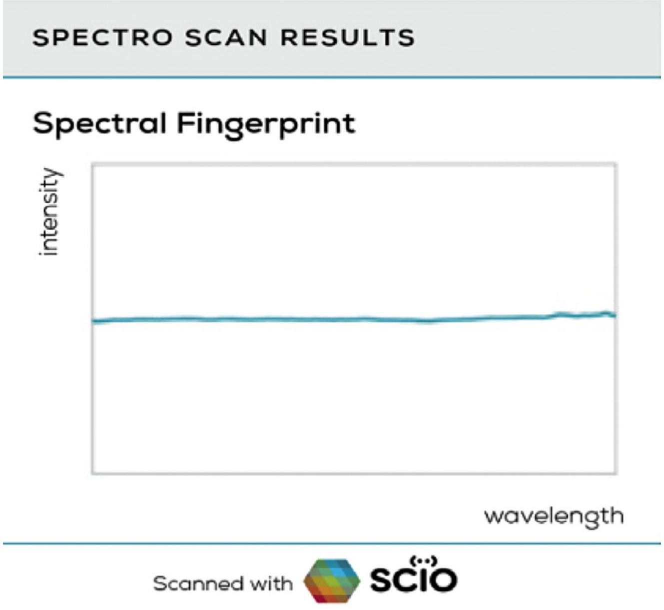

Figure 8 Screenshot from the SCiO Pocket Molecular Sensor app: the diagram shows the spectral fingerprint of potassium chlorate, measured by the author

well the students worked, the SCiO will identify it as one of several different substances that show little to no absorption in the part of the spectrum measured.

Expect a lot of classroom discussions about who has the right answer and what this means in terms of the safety of the substance. Many students will trust the 'authority' of the device instead of considering the limitations of the method. By comparing it with the other eight substances and studying the safety sheets, clever students will identify it as potassium chlorate, which has three pictogram-style safety warnings and should not be handled by the students themselves (see safety note below). It could have been just ordinary table salt (sodium chloride), which was one of the known provided substances in the lab, but this can be excluded through reasoning aided by the CLEAPSS *Student Safety Sheets*.

Students usually come to different conclusions, with some analysing the data presented logically and therefore identifying the unknown substance as the hazardous chemical that it is, whereas others do not trust the devices or their own investigation. For a chemistry teacher, there is only one way to convince the students who did not come to the right conclusion: let's prove it, and let the proposed chemicals react together, both the unknown substances and a sample of the known ones. However, do

Safety: Students are normally not allowed to handle potassium chlorate (see CLEAPSS, 2019b). The students should not touch the unknown substances, only point towards them with the spectrometer, while under supervision of a teacher. Herein lies a big advantage of the non-invasive spectrometer: it obviates the need for the students to handle the chemicals.

not blend undiluted sugar with potassium chlorate and follow CLEAPSS safety guidelines (2019b and 2019c)!

4. Testing the chemicals to verify the result

(Optional for the case where three unknown substances were spilt.)

Chemistry teachers know what happens when mixing diluted sugar and potassium chlorate. These are effectively the same substances as used in 'the growling gummy bear' experiment, also known as 'the screaming jelly babies', a spectacular demonstration experiment (CLEAPSS, 2019c). In the jelly babies experiment, potassium chlorate serves as a strong oxidiser, which oxidises the sugar component of the jelly baby. The result is the rapid production of gases (carbon dioxide and water), which creates the noise and smoke (Figure 9).

Conclusion

After working through this sequence, even the most doubtful student will realise that carrying out a risk assessment was no joke, but a necessary part of laboratory work, and that the use of NIR spectroscopy helped them to work as chemical detectives with real-world substances. Therefore, I would argue that the time to use NIR spectroscopy in the science classroom has technically come, even if the devices are still too expensive for most schools. This is likely to change in the near future, with the integration of NIR sensors, and eventually sensors that can measure a broader spectrum, directly into smartphones, as some manufacturers have already demonstrated. Box 1 lists advantages and disadvantages we encountered when using this mobile NIR spectrometer.

Box 1 Pedagogical advantages and disadvantages of using the SCiO mobile NIR spectrometer

(Note that a technical analysis of the SCiO has been carried out by others, e.g. Sparkfun, 2019.)

Advantages

1 Student engagement: state of the art mobile devices rule!

2 Making chemistry visible: inquiry with real devices that may be usable in a lot of contexts, even out-of-classroom settings.

3 The limitations of the device can be used didactically to enhance critical thinking and awareness of sources of error.

4 Even if the consumer edition of SCiO is planned as a black box and used as that by us with lower grades, the device can be used as a nice starting point for inquiry-based teaching, motivating the students to learn about related topics such as radiation, analysis and health and safety.

5 If you are highly motivated, it is possible to buy a developer's licence to develop your own sophisticated applications, but we have not tested this option in the classroom.

6 Devices such as the SCiO present an opportunity to create new teaching sequences or analyse learning processes in high-tech learning environments. We have other teaching projects, for example, an interdisciplinary teaching unit in middle school, where students analyse food items with SCiO in the science class and then cook a meal with them in their food and health lesson.

7 This brings us to the last benefit. Polyethylene, which is one of the polymers often used in packing of food items, does not show absorbance in the near-infrared part of the spectrum. Consequently, many of the health and safety concerns around hygiene and potentially hazardous chemicals can be addressed by analysing substances through transparent packaging.

Disadvantages

1 If not discussed properly, students may assume the SCiO is a universal detector, but it is not. Technically and theoretically, it is rather a chance for students to handle a 'near-scientific' apparatus, even if it shows astonishingly consistent results for a number of organic substances. It cannot cover inorganic substances without covalent bonds such as NaCl, as they do not absorb frequencies in the near-infrared. An important point in our case!

2 The company producing the SCiO is not transparent about the limitations discussed above. Ideally, the 'spectral fingerprint' should include labelling of the wavelengths. With respect to science teaching, it would be nice if the term 'intensity' (*y*-axis, Figure 5) was explained as well. The 'intensity' shows normalised and processed data from the measured diffuse reflectance of a substance in the near-infrared spectrum, including a mathematical derivation.

4 Handling the device: the SCiO should be in its cover, but the cover is both very slippery and fixed to the device by rather weak magnets. The cover cannot be permanently fixed to the device as it needs to be taken out to charge and to calibrate. My colleague had the idea of wrapping the cover with sports tape, which makes it easier to hold, especially for younger students (Figure 4).

5 One spectrometer still cost about \$300 (≈ £235), when we bought a class set of 10 pieces, which means that it is not affordable for many schools. One solution may be collaborating with a nearby science centre or other institutions that buy a class set and lend it to schools, as we do. However, technology is moving forward fast, with major manufacturers currently working on integration of NIR sensors into smartphones, which will make these more affordable and universally available.

Figure 9 Testing the chemicals that were analysed by the students (NB: safety first, read CLEAPSS, 2019b,c)

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