Mass Spectrometry Basics for Young Students:

An Interactive Laboratory Tour

Julia H. Jungmann, Nadine E. Mascini, Andras Kiss, Donald F. Smith, Ivo Klinkert, Gert B. Eijkel, Marc C. Duursma, Berta Cillero Pastor, Kamila Chughtai, Sanaullah Chughtai, Ron M. A. Heeren*

FOM-Institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

Running title: Outreach: MS basics for young students

Keywords: mass spectrometry, ions, charged particle manipulation, building blocks of matter, science education, open day, open house, outreach

* Address reprint requests to Ron M. A. Heeren, FOM-Institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands, Telephone: +31-20-7547100, Fax: +31-20-7547290, E-mail: heeren@amolf.nl

Abstract

It is imperative to fascinate young children at an early stage in their education for the analytical sciences. The exposure of the public to mass spectrometry presently increases through the common media. Outreach activities can take advantage of this exposure and employ mass spectrometry as an exquisite example of an analytical science that children can be fascinated for. The presented teaching modules introduce young children to mass spectrometry and give them the opportunity to experience a modern research laboratory. The modules are highly adaptable and can be applied to young children from the age of 6 years to 14 years. In an interactive tour, the students explore three major scientific concepts related to mass spectrometry; the building blocks of matter, charged particle manipulation by electrostatic fields and analyte identification by mass analysis. Also, the students carry out a mass spectrometry experiment and learn to interpret the resulting mass spectra. The multistage, inquiry-based tour contains flexible methods which teach the students currentday research techniques and possible applications to real research topics. Besides the scientific concepts, laboratory safety and hygiene are stressed and the students are enthused for the analytical sciences by participating in "hands-on" work. The presented modules have repeatedly been practiced during laboratory open days but are equally suitable to complement (early) high school science classes when combined with a laboratory visit.

Introduction

Mass spectrometry (MS) is an analytical technique which identifies compounds based on the atomic sample composition of the molecules and their charge state [1]. Therefore, "blind" analysis of unknown samples is possible since MS does not require detailed prior knowledge of the sample composition. Ideally, the chemical identification by MS is not limited by analyte pre-selection as, for example, in analysis techniques based on fluorescent or radioactive labeling. This bears the advantage that the analysis technique itself does not make any functional changes to the molecules under investigation. The applications of mass spectrometry range from among others environmental analysis, isotope dating and tracking, trace gas analysis, proteomics, lipidomics, metabolomics to clinical applications and forensics.

MS is a particularly interesting and valuable analytical technique to share with children and young science education students. When explaining mass spectrometry, i.e. "finding out what something is by weighing it", the concept of "the building blocks of matter" is introduced (i.e. the elements and molecules). The specificity of a building block's mass in relation to its identity is explained. Also, possible fields of application of MS (which the participants might already be familiar with through the common media, e.g. crime scene investigation, food allergies etc) are discussed. Further, the need and concept of electrostatic fields for the manipulation of charged particles through the mass spectrometer is explained.

Laboratory experiences for children and early science students are generally accepted as a

3

valuable learning tool [2]. In particular, it has been proven an effective learning and teaching strategy to give students the opportunity to actively explore and experience the course content of their science classes [3]. Additionally, it is recognized that a laboratory visit will reinforce scientific concepts that have been studied in a class room context [4], which indicates the relevance of the presented teaching modules to complement (early high) school science education. Additionally, the scientific curiosity of young children can be triggered and stimulated by open house laboratory days that are specifically tailored to young children. Akerson and co-workers [5] have demonstrated the importance to start science education in early childhood years and proved that the children are well capable of understanding complex scientific concepts when appropriately presented. Benkinson and Chen have successfully introduced proteomics to the classroom [6].

In this paper, we report on three teaching modules which together introduce the concept of mass spectrometry to children of the age 6 to 14. The modules are designed to convey a complex analytical technique to the pre- and/or early-science education level. The main goals of the modules are threefold: to convey the concept of MS to young children/early science students, to enthuse children for the analytical sciences and to familiarize them with a laboratory environment at an early stage. The presented teaching tour is suitable for both (MS/chemistry) laboratory open days or science class<u>es</u> in combination with a laboratory visit (see Box 1 for the student learning outcomes).

Box 1: Student learning outcomes.

At the end of the three modules, participants

- Understand the concept of mass spectrometric analysis: Analyte identification via analyte molecular mass.
- Understand that charged particles can be manipulated by electrostatic forces.
- Understand the basic elements of a mass spectrometric experiment: Sample preparation, mass analysis and data interpretation.
- Are introduced to laboratory hygiene and safety.
- Know several areas of application of mass spectrometry.

Methods

Teaching Format

The teaching format is a multistage, exploratory tour for children, "Weighing is knowing!".

The targeted age group is from 6 to 14 years (adjustments are required to fit the respective age group). Modules have been designed for 8-10 children per group. The three module tour is suitable for more students if the class is divided into multiple groups of 8-10 students. The entire tour takes about 45 minutes to one hour.

Description of the teaching program: The interactive laboratory tour

Module 1: Analyte idenfication via analyte mass.

GOAL: Explain the link between mass and analyte ("building block") identification.

WHAT: An interactive game/competition.

In Module 1 of the tour, the concept of building blocks of matter and analyte identification via analyte mass, i.e. the core concept of mass spectrometry, is developed interactively with the children. For a setting in a (MS) lab facility, the explanation is structured as follows: The children are welcomed to the lab by the teacher. He/she announces that the students will learn what the research group does in their laboratory. Also, the class is strongly encouraged to ask questions along the way. The initial welcoming session is intended to trigger the students to think about how to investigate small "things". This discussion is steered towards the concepts of building blocks of matter and mass spectrometry, i.e. "looking" at the building blocks of matter by "weighing" them. The introduction ends with a rationale describing why it is important to analyze unknown samples by mass spectrometry, which is easily related to the daily life of the students. The methodology of this introductory session is provided in Box 2.

After this introductory discussion, an interactive game further illustrates the concept of analyte iden<u>ti</u>fication via analyte mass. The methodology and materials for this game are provided in Box 3 and the Supplementary Materials 1, respectively.

The activities of Module 1 have been conducted several times with students of different age groups (6-14). The activities of Module 1 do not require any prior science education. However, dependent on the age and the level of previous science education, the activity and terminology can easily be tailored to the prior knowledge of the children. The activity is most suitable if the group of 10 students is divided into 3-5 teams during the game. The activity can be scaled towards larger classes if the materials are scaled accordingly. The activities of Module 1 take about 10-15 minutes to complete.

6

Box 2: Instructions and sample questions to Module 1: Analyte idenfication via analyte mass.

- How to investigate small "things". To start, the students can be challenged with questions: "Does anyone have an idea how you can look at things that are so small that you can barely or even not see them with your eyes?" Many kids think about magnifying glasses or maybe a microscope that they have used in early science education classes. The teacher/researcher points out to them: "This works well for many small things. However, the "things" that are looked at and have to be analyzed in the laboratory here are so small that they cannot be seen with the naked eye at all and even a microscope or magnifying glass will not do the trick. In a mass spectrometry laboratory, there is yet another method to "look" at things that cannot be seen with the naked eye. Even if we cannot see these things, we can "weigh" them with a special type of scale balance."
- **The building blocks of matter.** In simple terms, the teacher explains that: *"Everything around us consists of very small building blocks "atoms" and clusters of building blocks "molecules". Atoms and molecules are so small that we cannot see them. The different building blocks of different materials have a different mass."*
- Analyte identification: The teacher asks the students if they have an idea about a technique that could figure out which building block is which. Possibly the students have grasped the concept of analyte (=building block) identification by mass (=weighing) already and will point this out. If not and/or to illustrate the point of analyte identification by mass, the teacher can take two boxes and put a feather in one and a small rock in the other. Then, the lid is closed such that from the outside of the boxes it is impossible to find out what is inside by visual inspection. The teacher asks the students how they would find out about what is in the box and helps to develop the concept of analyte identification by mass spectrometry. Now it becomes clear that: "If you can weigh a sample, you can figure out what it is! We call this technique "identification"." The small feather-rock experiment naturally leads to the interactive game that is performed in the next stage of the module.

• Why bother? What is mass spectrometry good for?

Finally, it is important to motivate why analyte identification by mass spectrometry is relevant to the society and the students. The teacher asks the group if they have any idea why the researchers look at unknown samples by mass spectrometry. *"Why do we want to figure out what is inside a sample?"* Some students might have an idea; possible examples that trigger the students' interest are food control (lactose intolerance, nut allergy etc), medical diagnosis or crime scene investigation.

Box 3: Instructions for the interactive game, sample questions and explanations (Figure 1).

- Models of the building blocks of matter. The teacher encourages the students to think about the concept of building blocks of matter (Figure 2a): "Let's look at the building blocks! The building blocks are very small but we have made some models for you." The teacher shows them the building block models (toy molecular models) and reminds them that everything around them consists of the building blocks. "No matter how big something is. It's made of small building blocks. And for each building block, we know the mass."
- Idea behind the game. The teacher introduces the game. "In this game, you can figure out the identity of an unknown sample by weighing it. And, this is what we do in our laboratory here. We have a box with some kind of sample in it but we have no idea what's inside! We then use our laboratory equipment to find out what building blocks are inside the sample. We do that by weighing the building blocks. Really, our machines in the laboratory are not more than big, fancy scale balances."
- **The game.** The teacher divides the class into groups of 2 (to maximally 3) students that will work together. "Now, you get to figure out what's inside the box." On one table, there are several numbered boxes (see materials for the preparation of this game). The teacher points out that: "Every box represents one type of molecule (=one material), which has a unique mass. Each box contains one of the molecules that you see here (teacher points to the models of the molecules (Figure 2a); see materials section). From just looking at the box, we do not know which molecule is inside. All boxes look the same. A good way to figure out what is inside the box is ...?" The students realize "...to weigh the box!" Every group takes a box from the table and weighs it on a scale balance (Figure 2b). Using the mass from the scale balance, the students come back to the table with the molecular models and "identify" which molecule was in the box (Figure 1). The students can check their result by opening the box (Figure 2c); inside the box there is a photo of the molecule. "Did it work out?" The students are instructed to identify which molecule is inside several of the boxes by weighing them. The teams compete in who can identify all molecules in the shortest time.
- Wrap up. The teacher points out that: "Now you know how to figure out which building blocks are inside an unknown sample: By weighing it!" Now it is time to learn how researchers work with the molecules in the laboratory.

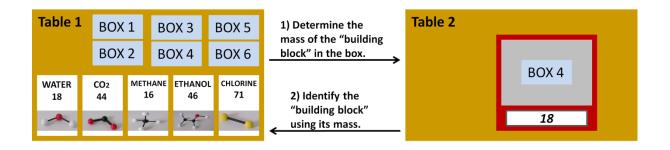


Figure 1. Interactive game to illustrate the concept of analyte identification by mass spectrometry.



Figure 2. Photos of the interactive game of Module 1. A group of students explores the concept of analyte identification by mass spectrometry during a laboratory open house day.

Module 2: Mass spectrometry to identify very small "objects" by mass and the use of electrostatic fields

GOAL: Explain that a mass spectrometer separates very small "objects" of different mass; explain that mass separation relies on charged particles.

WHAT: (Interactive) demonstration on charge/static electricity.

Module 2 of the tour shows that mass spectrometry relies among others on the use of electrostatic fields to manipulate the charged analytes of interest. The concept of electrostatic fields is illustrated during an interactive demonstration. Electrostatic fields are conceptually compared to "forces" (like wind) and mass separation by means of electrostatic fields is demonstrated. The methodology of the demonstration is outlined in Box 4 and Figure 3; the required materials are described in the Supplementary Materials 2.

The demonstration of Module 2 can be carried out with the entire class or in smaller groups to increase the interaction with the researchers. The Module takes about 10 minutes.

Box 4: Instructions for the interactive demonstration on the use of electrostatic fields for mass spectrometric analysis; sample questions and explanations.

- Introductory questions. The teacher asks the students: "How can we use a "force"
 (something invisible) to separate things?" Even with prior science education this is a
 challenging concept to grasp. The teacher can guide the class with an analogy:
 "Imagine two balls lying on the beach: a soccer ball and an air-filled beach ball. If wind
 comes up on the beach, which ball will fly away more readily?" The class immediately
 realizes that the beach ball will fly off more easily. The teacher steers the class to
 thinking about: "Why does the beach ball fly away and not the soccer ball?" The class
 easily will realize that this is the case: "Because it is lighter!" The teacher explains: "The
 wind blows equally strong on both balls but its strength (=the force) has a different
 effect! Thus, with the invisible "wind force", we can separate different masses!" The
 introductory questions convey the concept of mass separation by a (n invisible) force
 and set the stage for moving on to the concept of electrostatic forces.
- Electrostatic forces. The teacher leads the conversation towards electrostatic forces: "There are more invisible forces. Maybe you experienced some of them before. For instance, if you rub a rubber tube with a piece of cloth, you can lift up your friend's hair, or styrofoam pieces or pieces of paper." The teacher asks a student to rub a rubber tube on his/her pullover and then the student can attract some small pieces of paper or his/her friends' hair (Figure 4a). The teacher points out: "that you can "pull" on things with electrical forces."
- *Electrical forces and mass spectrometry.* After this demonstration, the teacher links electrostatic forces and mass spectrometry: *"That's also what we do in a mass spectrometer! We push and pull on particles using electrostatic forces."*
- Demonstration. The goal of this demonstration is to show the separation of different • "masses" with electrical forces (Figure 3 and 4b). The teacher can introduce mass separation with a question: "I can lift up your hair with the Perspex rod but when I try to lift the table it won't move ... Why? The table and the hair have different masses!" A dedicated setup is prepared to "mass separate" two liquids. In this setup (Figure 3), tap water and viscous sugar syrup are each pumped through hoses hanging on a stand. When they are pumped through the hoses, both the water and the syrup make it to the end of the hose on the stand and fall straight down into a bucket on the table (Figure 3a). However, if we place a metal sphere connected to a Van de Graaff generator next to it and charge up the sphere, we can make "electrical wind" (forces). Now, the water and the syrup droplets are attracted towards the metal sphere (Figure 3b and 4c)! The teacher points out: "The charged sphere can pull on the water droplets just like we pulled on your hair after we charged up the Perspex rod by rubbing it on your pullover!" The teacher asks the students to watch carefully what is happening now: "The water and the syrup are attracted towards the charged sphere and they fall into different buckets!" The students observe that the water droplets fall into the bucket closer to the sphere and the syrup falls into the next bucket closer to the hoses, i.e. water is "lighter" than syrup! The teacher wraps up by leading the students to realize that: "We have separated the water and the syrup (the different masses!) with electrostatic forces "

11

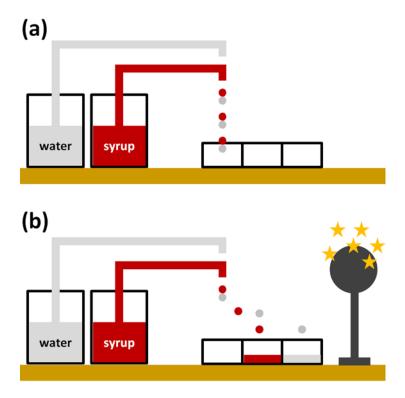


Figure 3. Demonstration to show mass separation by means of electrostatic fields. Water and viscous sugar syrup are pumped out of a beaker into a hose. (a) If no fields are applied both the water and the syrup fall down into the collecting tray. (b) If the Van de Graaff generator charges the metal sphere (indicated by stars), the droplets are attracted towards the sphere. The water is "lighter" than the syrup and will be pulled closer to the sphere. The water and the syrup fall into different segments of the collecting tray, i.e. mass separation by means of electrostatic forces.



Figure 4. Photos of the demonstration of Module 2. (a) The students play with static electricity; they rub a Perspex rod on their pullovers and then can lift up their hair. (b) The teacher explains the "mass separation setup". (c) "Mass separation", i.e. water and syrup are separated, by electrostatic fields.

Module 3: "Real" mass spectrometry in action.

GOAL: Show the students a "real" mass spectrometry laboratory; identification of compound by mass spectrometry; laboratory experience.

WHAT: (Interactive) demonstration, mass identification game.

In Module 3 of the laboratory tour, the students are brought inside an analytical chemistry laboratory where the concepts developed in Module 1 and Module 2 are put into practice. Generally, a MS experiment consists of three distinct parts: Sample preparation, mass analysis and data analysis/interpretation. In the last stage of the exploratory tour, the students participate in a "real" MS experiment and hence "hands-on" experience all three parts of the MS experiments.

Importantly, Module 3 takes the class into an analytical chemistry laboratory and hence offers the opportunity to introduce basic laboratory safety and chemical hygiene. First, the

students put on lab coats and the teacher can discuss that laboratory coats protect both the researchers working in the laboratory and prevent the contamination of a "clean" working environment (Figure 5a). Later during the mass spectrometry measurements, gloves are used. Second, the class is introduced to the laboratory equipment. The teacher shows them the mass spectrometers and points out that these machines are our "scale balances" for molecules: *"They are called mass spectrometers because they measure the masses of different compounds."* After the class is settled in the lab, a hands-on mass spectrometry experiment is performed in which the students are familiarized with sample preparation, mass analysis and the analysis of the experimental results. The methodology and procedure of the experiment and the required materials are given in Box 5, Figure 5 and the Supplementary Materials 3, respectively.

The introduction to laboratory safety and laboratory hygiene (as well as dressing into laboratory coats) takes about 5 minutes for the entire class. The brief introduction to the laboratory equipment and mass spectrometers can be tailored to the level of the prior knowledge of the class and can hence take 5-10 minutes. The mass spectrometry experiments take about 10-15 minutes for about 3 rounds of analysis. This step can be repeated depending on the size and enthusiasm of the class.



Figure 5. Mass spectrometry experiment in the laboratory. (a) The group is dressed in laboratory coats and welcomed in the lab. The teacher introduces the equipment and explains the procedure of the experiment/game. (b) A volunteer chooses one beverage, drinks a couple of sips and then spits into a cup. (c) A researcher prepares the saliva sample for analysis together with the student and introduces it in the mass spectrometer. (d) Data interpretation: The students look at the saliva spectrum and compare it to "standard" spectra of the beverages. Box 5: Methodology and procedure of the "hands-on" mass spectrometry experiment.

- Setup/idea of the experiment. One student is picked out of the group (volunteer). This student is separated from the group and chooses one out of several beverages (coffee, cola, lemonade etc, Figure 5b). The student does not reveal to the class which drink he/she chose. The student drinks some of the beverage and then spits into a plastic cup, i.e. the student provides a "saliva sample". The sample is prepared for mass spectrometric analysis and then injected into a mass spectrometer (Figure 5c). The class is provided with the resulting saliva spectrum and spectra of the "pure analytes" (=standards), i.e. a coffee, cola, lemonade etc spectrum. Each of the standard spectra shows a peak characteristic for the drink. The class can identify which drink was present in the saliva by comparing the saliva spectrum to the standard spectra (Figure 5c).
- Details of the mass spectrometric analysis. The saliva sample is diluted in methanol (1:1, by volume). Then, the sample is electrosprayed into the mass spectrometer. Depending on the age of the students, a scientist can perform the sample preparation and introduce the sample into the spectrometer, or the student can perform these tasks under supervision. Importantly, here laboratory hygiene (lab coat, gloves) and laboratory safety ("Wear gloves and goggles when handling chemicals! Be carefullcareful what you touch!") can be stressed. The class can watch the spectrum build up online on the computer screen.

Wrap-Up: Relationship with the research in the host laboratory.

GOAL: Relate the newly learned concepts to present-day research topics of the host laboratory.

WHAT: Discussion.

At the end of the laboratory tour concludes the teaching unit by relating the newly learned concepts to the state-of-the-art research of the research laboratory. What is the research used for? And why is this research important. The teacher can relate mass spectrometry experiments as just performed by the students, for instance, to forensic research ("crime scene investigation" (CSI)), food control, disease studies or other applications that the participants might be familiar with.

The concluding discussion takes approximately 5 minutes and can be adjusted to the age of the students.

General remarks.

The laboratory should be clean and safe. The students should not be exposed to hazardous substances or unsafe equipment. Instead of one teacher leading the activity, it is also possible that every module is conducted by a different researcher stressing the fact that mass spectrometry based research is team work.

Conclusion and Outlook

The presented teaching modules have repeatedly been practiced with children in our laboratory –particularly for open days and high school tours at FOM-AMOLF. This "kids tour" is perceived as a "great hit" by teachers, scientists and most importantly the children themselves! We have hosted many groups of children between the age of 6 years to 14 years and are pleased to observe that the basic concepts of mass spectrometry, i.e. the building blocks of matter, charged particle manipulation by electrostatic fields and analyte identification by mass analysis, are rapidly understood and applied by the participants. Also, the laboratory experience (lab coats, gloves, the noise of the pumps on the spectrometers etc) enthuses the participants and triggers many good questions.

In our experience, most children have been exposed to mass spectrometry through the media (mainly science-centered drama series on television) and easily relate this field of analytical chemistry to forensics, food monitoring, the health sector etc. Hence, mass spectrometry is a very suitable example to fascinate young students for the technical sciences.

We encourage you, our colleague mass spectrometrists and analytical scientists, to share your enthusiasm for research with children! The teaching modules presented here give an indication of what type of activities are feasible and fun for both research laboratory open days, high school class visits or to complement (early) science education. We found one of the participating children asking: "Can I have one of those mass spectrometers to play with at home?". An immediate challenge for the next generation mass spectrometrists: small, affordable MS systems included in high school science education and introduced into the

18

homes of many. After all, we all would like to monitor and maintain health and a healthy living environment.

Acknowledgements

This work is part of the research program of the "Stichting voor Fundamenteel Onderzoek der Materie (FOM)", which is financially supported by the "Nederlandse organisatie voor Wetenschappelijk Onderzoek (NWO)".

References

1. De Hoffmann, E.; Stroobant, V. Mass Spectrometry: Principles and Applications, 3rd ed.; Wiley and Sons; 2007.

2. Downing, E. Supervised study and the science laboratory. School Review. 1917, 25, 646-651.

American Association for the Advancement of Science, Science for all Americans: A project
2061 report on literacy goals in science, mathematics, and technology. Washington D.C.,
AAAS, 1990.

4. Angelini, R.; Ferreira, J. S.; Carmo Araujo, C. S.; Carvalho, A. R. Effect of Outdoor and Laboratorial Environment Science Activities on Middle School Students Understanding on Conservation. Natureza & Conservacao, 2011, 9, 93-97.

5. Akerson, V. L.; Valarie, L.; Buck, G.A.; Donnelly, L. A.; Nargund-Joshi, V.; Weiland, I. S. The Importance of Teaching and Learning Nature of Science in the Early Childhood Years, J. Sci. Educ. Technol. 2011, 20, 537-549.

6. Benskin, J.; Chen, S. Proteomics in the Classroom: An Investigative Study of Proteins in Microorganisms. Am. Biol. Teach. 2012, 74, 237-242

Figures

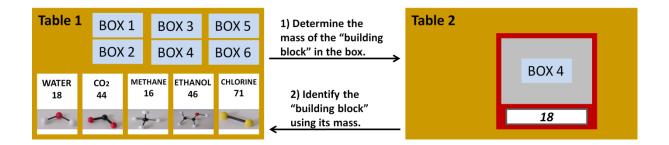


Figure 1. Interactive game to illustrate the concept of analyte identification by mass

spectrometry.



Figure 2. Photos of the interactive game of Module 1. A group of students explores the concept of analyte identification by mass spectrometry during a laboratory open house day.

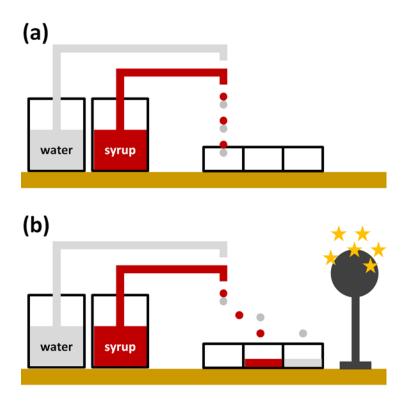


Figure 3. Demonstration to show mass separation by means of electrostatic fields. Water and viscous sugar syrup are pumped out of a beaker into a hose. (a) If no fields are applied both the water and the syrup fall down into the collecting tray. (b) If the Van de Graaff generator charges the metal sphere (indicated by stars), the droplets are attracted towards the sphere. The water is "lighter" than the syrup and will be pulled closer to the sphere. The water and the syrup fall into different segments of the collecting tray, i.e. mass separation by means of electrostatic forces.



Figure 4. Photos of the demonstration of Module 2. (a) The students play with static electricity; they rub a Perspex rod on their pullovers and then can lift up their hair. (b) The teacher explains the "mass separation setup". (c) "Mass separation", i.e. water and syrup are separated, by electrostatic fields.



Figure 5. Mass spectrometry experiment in the laboratory. (a) The group is dressed in laboratory coats and welcomed in the lab. The teacher introduces the equipment and explains the procedure of the experiment/game. (b) A volunteer chooses one beverage, drinks a couple of sips and then spits into a cup. (c) A researcher prepares the saliva sample for analysis together with the student and introduces it in the mass spectrometer. (d) Data interpretation: The students look at the saliva spectrum and compare it to "standard" spectra of the beverages.