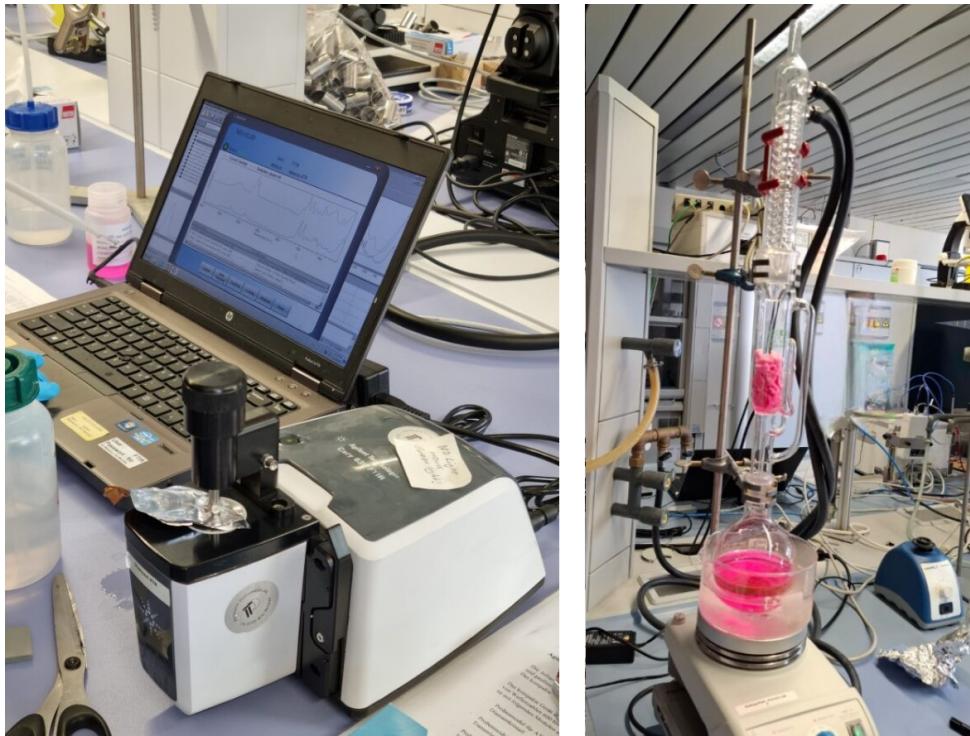


## Lab report

### Analysis and identification of Plastics by Soxhlet extraction and ATR-IR



### Principle of Sustainable Environmental Systems

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# Contents

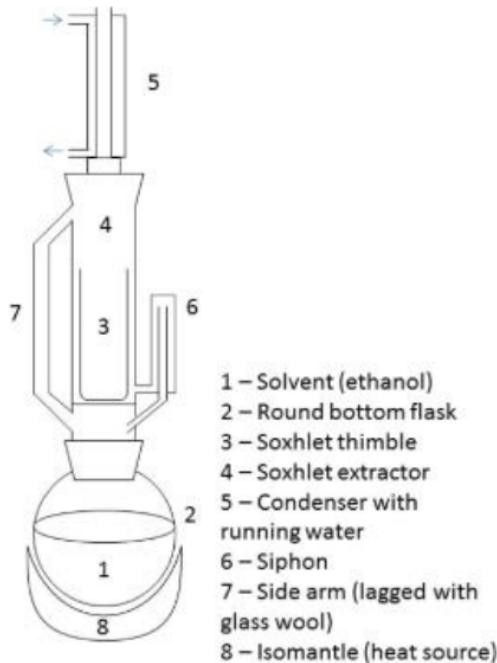
<b>1</b>	<b>Introduction</b>	<b>3</b>
1.1	Soxhlet extraction . . . . .	3
1.2	Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-IR) . . . . .	3
<b>2</b>	<b>Materials and Methods</b>	<b>4</b>
2.1	Material for Soxhlet extraction method . . . . .	4
2.1.1	Rhodamine B . . . . .	4
2.2	Material for ATR-IR . . . . .	4
2.3	Procedure . . . . .	4
2.3.1	Soxhlet extraction . . . . .	4
2.3.2	ATR-FTIR . . . . .	5
<b>3</b>	<b>Results</b>	<b>6</b>
3.1	Selection of the Soxhlet solvent . . . . .	6
3.2	Soxhlet extraction . . . . .	6
3.3	ATR-FTIR analysis . . . . .	6
3.3.1	Sample 1: White foam . . . . .	7
3.3.2	Sample 2: Inside of a Twix bar wrapper . . . . .	8
3.3.3	Sample 3: Outside of a Twix bar wrapper . . . . .	9
<b>4</b>	<b>Discussion</b>	<b>10</b>
4.1	Litter in Horw . . . . .	10
4.1.1	Questions . . . . .	11
4.1.2	Availability of bins . . . . .	11
4.1.3	Regual cleaning and maintenance . . . . .	11
4.1.4	Public culture . . . . .	11
4.1.5	Invisible trash . . . . .	11
4.2	Soxhlet extraction: results interpretation . . . . .	12
4.2.1	Questions . . . . .	12
4.3	ATR-FTIR analysis: results interpretation . . . . .	12
4.3.1	Questions . . . . .	12
4.3.2	Methodology . . . . .	13
4.3.3	Identification . . . . .	13
4.3.4	Impact on the environment . . . . .	13
<b>5</b>	<b>Conclusions</b>	<b>14</b>
5.1	Field observation and Waste management . . . . .	14
5.2	Characterization of waste . . . . .	14
5.3	Methodological assessment and Future work . . . . .	14
<b>A</b>	<b>Appendix</b>	<b>15</b>
A.1	Inventory of samples collected . . . . .	15
A.2	ATR-FTIR analysis . . . . .	18

# 1 Introduction

Plastic is a material found in every environment, and its use is indispensable in everyday life, present in consumer products and industrial applications. However, plastics often contain additives that modify their properties, such as their appearance or performance. Analyzing and understanding the composition of plastics is essential for mitigating pollution and protecting nature so that their environmental hazards can be effectively minimized.

This experiment focuses on the extraction of admixtures from plastics and on the spectroscopic analysis of polymers in order to determine their chemical composition and the functional groups of the molecules. By combining these two techniques, it is possible to evaluate and study the environmental impact of polymers and their additives.

## 1.1 Soxhlet extraction



Soxhlet extraction is a chemical separation technique based on extraction cycles. The technique consists of the separation of soluble compounds from solid materials and relies on the differences in solubility between the analyte and the solid matrix; that is the portion of the sample that remains insoluble in the chosen solvent.

A Soxhlet extractor is composed of a round-bottom flask in which the solvent is boiled (1,2) heated up by an isomantle (8), a thimble (3) needed for holding the solid sample that contains the analyte to be extracted, which in turn is contained in the Soxhlet body (4). A siphon (6) and a side arm (7) connect the flask to the body, enabling the solvent circulation throughout the system.

A Soxhlet cycle is made up of solvent boiling, vapor condensation, percolation through the sample, and siphoning of the extract back into the boiling flask. A condenser with running water (5) is used to liquefy the rising solvent vapors and drip back onto the sample.

Figure 1: Soxhlet extractor components

## 1.2 Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-IR)

Fourier transform infrared spectroscopy (FTIR) consists of a broadband infrared source. To measure all frequencies simultaneously, the beam must first pass through an interferometer to encode the light (ScienceDirect Topics, 2025b). Afterwards, the infrared light is sent to an ATR extension to probe the sample.

Attenuated total reflection extension (ATR) consisting of a crystal with a high refractive index (ScienceDirect Topics, 2025a). The extension holds the sample in place with maximum contact to the crystal.

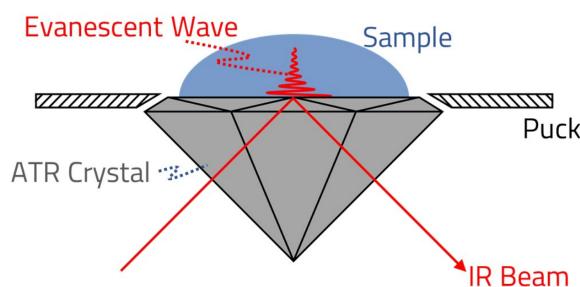


Figure 2: Graphical representation of a single bounce ATR (Specac Ltd., 2024)

The infrared beam from the FTIR source arrives and enters the crystal at a specific angle, is internally reflected many times, and an evanescent wave forms. The evanescent wave will penetrate out of the crystal and into the sample at a depth of around 0.5 - 2 micrometers (ScienceDirect Topics, 2025a). Chemical bonds from the sample are excited at specific frequencies and absorb energy.

Finally, a detector collects the returning beam, and a Fourier Transform is performed to calculate the final absorbance graph, visually showing at which frequencies the material has been absorbing energy (ScienceDirect Topics, 2025c).

## 2 Materials and Methods

### 2.1 Material for Soxhlet extraction method

- Soxhlet extractor body
- Glass reflux condenser
- Round-bottom flask (RBF)
- Hot plate with heating controller
- Support and clamps
- Cooling water supply and tubing (secure with clamps)
- Polymer sample impregnated with rhodamine B (record mass)
- Solvents

#### 2.1.1 Rhodamine B

Rhodamine B is an organic molecule that exists as the chloride salt, and it is notable for its intense fluorescence and use in tracing and dye applications (National Center for Biotechnology Information, 2025). It is widely used in fluorescence microscopy and as a tracer in hydrodynamic studies because of its bright emission and sensitivity to the environment.

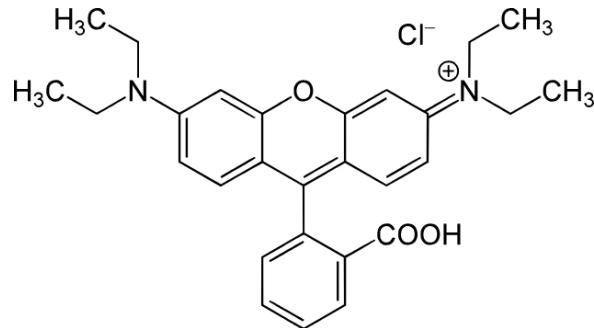


Figure 3: Rhodamine B

### 2.2 Material for ATR-IR

- Plastic samples
- Agilent Technologies Cary 630 FTIR Spectrometer
- Isopropyl alcohol

### 2.3 Procedure

The laboratory work was divided into two main phases: determining the most suitable solvent for the extraction of rhodamine B from a provided polystyrene-based plastic sample (matrix) using a Soxhlet extractor, followed by the identification of plastics and their functional groups in samples collected along the street between the HSLU T&A building and the Lucerne Lake.

#### 2.3.1 Soxhlet extraction

In this experiment, additives were extracted from a polystyrene-based plastic sample containing rhodamine B using a Soxhlet extractor, then further identified and characterized. Before the extraction, a small piece of the polymer was tested with different solvents to select one that dissolved the dye but did not dissolve the plastic matrix. Once a suitable solvent had been identified, the required volume was measured and transferred into a clean round-bottom flask (RBF), filling half of its volume. The mass of the polymer sample was recorded, and the sample was placed into the extraction thimble, which was then positioned inside the Soxhlet body. The Soxhlet extraction was then carried out using a standard assembly consisting of a round-bottom flask (RBF),

a Soxhlet body, and a water-cooled reflux condenser. The RBF, filled with the selected solvent, served as the boiling reservoir, while the polymer sample was placed in an extraction thimble positioned within the Soxhlet chamber. The system was heated to establish a gentle, continuous reflux. Under these conditions, solvent vapor is condensed in the condenser and percolates through the sample in repeated cycles. Each siphon event returns the enriched solvent to the RBF, enabling continuous extraction as the dye progressively accumulated in the boiling flask.

### 2.3.2 ATR-FTIR

The composition of two different pieces of plastic waste was identified using the Agilent Technologies Cary 630 FTIR Spectrometer. Before the samples were measured, the crystal was thoroughly cleaned with isopropyl alcohol. This was followed by a background measurement to calibrate the baseline. The chosen sample was then placed under the spectrometer, and a measurement was recorded. Using the built-in library of reference materials, the most likely match was chosen and plotted next to the measured sample. In the results given by the spectrometer, the most likely match appears as a blue line, while the measured sample appears as a red line. As the spectrometer can only measure one side of the sample, if necessary, the sample was flipped, and the other side was measured due to possible differences in materials. Finally, before proceeding to the next measurements, the crystal was always cleaned using isopropyl alcohol.



Figure 4: Measurement procedure for the sample “Twix inside”



Figure 5: Measurement procedure for the sample “Twix outside”

Out of the 17 trash samples collected, the Twix wrapper and the white foam were chosen as they were found next to the shoreline of the lake, where their potential environmental impact is greatest. The location of these samples can be seen in Figure 13 under the points 12 and 13, next to the Seerosenplatz.

### 3 Results

The following section reports the results obtained from Soxhlet extraction and ATR-FTIR analysis.

#### 3.1 Selection of the Soxhlet solvent

In order to determine the best solvent for the Soxhlet extraction of the rhodamine B from the polystyrene-based samples, four candidate solvents were tested and categorized according to their properties and their effectiveness on the matrix and the dye:

Table 1: Candidate solvents properties and effectiveness

Solvent	Solubility of matrix	Solubility of dye	Boiling point [°C]	Toxicity	Polarity
Hexane	Insoluble	No extraction	69	High: neurotoxic	Non-polar
Diethyl ether	Slight swelling	No extraction	35	High: peroxide-forming	Low polarity
Acetone	Swelling	No extraction	56	Moderate: irritant	Moderately polar
Ethanol	Insoluble	Strong extraction	78	Low toxicity	Polar

#### Scales used

Matrix solubility: Insoluble – Slight swelling – Swelling – Partially soluble – Soluble

Dye solubility: No extraction – Weak – Moderate – Strong – Complete extraction



Figure 6: Result of the solvents effectiveness experiment

#### 3.2 Soxhlet extraction

Throughout the Soxhlet extraction, a progressive change in the appearance of both the solvent and the matrix was observed. At the beginning of the process, the ethanol in the round bottom flask looked completely colorless, and the polystyrene samples were brilliant pink due to the presence of rhodamine B. With the progression in the extraction cycles, the ethanol gradually stained due to the extraction of the additive in the sample, turning the solvent pinker. Simultaneously, the polymer-based sample reduced its color intensity every siphoning cycle. The experiment finished before the first cycle due to time constraints, nonetheless, assuming between 20 and 60 cycles, with a cycle duration of 5 to 10 minutes, the expected result is bright-pink colored ethanol due to the presence of dissolved rhodamine B in the solvent, and a bleached sample compared to its initial state.

#### 3.3 ATR-FTIR analysis

The results from the two different samples are listed, each with a picture of the sample, the measured absorbance graph (in red) compared to the reference graph from the library (in blue), and a table containing information about the functional groups and possible compounds. These were determined using the reference table provided in the lab (Table 5).

### 3.3.1 Sample 1: White foam

Sample 1 is a foam found in nature.



Figure 7: Collection of Sample 1

The sample has a white color and has a non glossy rough finish. It is quite squishy and soft. Small air pockets in the material make it foam like.

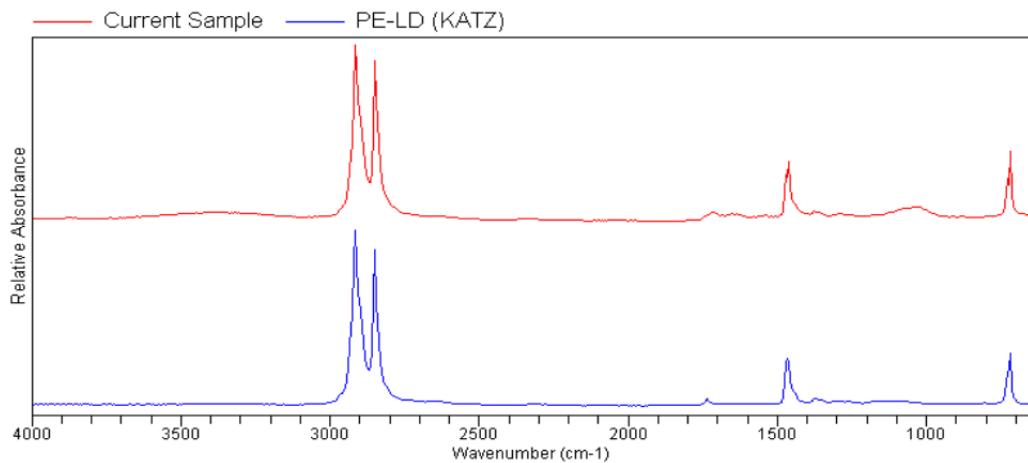


Figure 8: Sample 1 ATR-FTIR analysis

After the ATR-FTIR was done measuring the sample, it plotted an absorbance graph seen in Figure 8. It shows two sharp peaks around  $2900\text{ cm}^{-1}$ . Using Table 5, this cluster consists of Alkane and Methyleneether.

Furthermore, there are two smaller peaks at roughly  $1500\text{ cm}^{-1}$  and  $700\text{ cm}^{-1}$ , corresponding to Hydrocarbons/Esters and Monosubstituted Benzenes. The full list of data is shown in Table 2.

The blue graph matches the red graph neatly. The reference library suggested the sample is low density polyethylene.

Table 2: Sample 1 results

Peak [ $\text{cm}^{-1}$ ]	Functional groups	Possible compound
2900	$\text{CH}_3$ Valenz.	Alkane
2820	$\text{CH}_3$ Valenz.	Methyleneether
1480	$\text{CH}_3$ and $\text{CH}_2$ deform.	Hydrocarbons/ Esters
710	C — H Deform.	Monosubstituted Benzenes

### 3.3.2 Sample 2: Inside of a Twix bar wrapper

Sample 2 is a Twix bar wrapper found beside the railway in Horw.



Figure 9: Sample 2 during the analysis

The wrapper has two different textures. The inside looks silver and shiny. The material is quite sturdy.

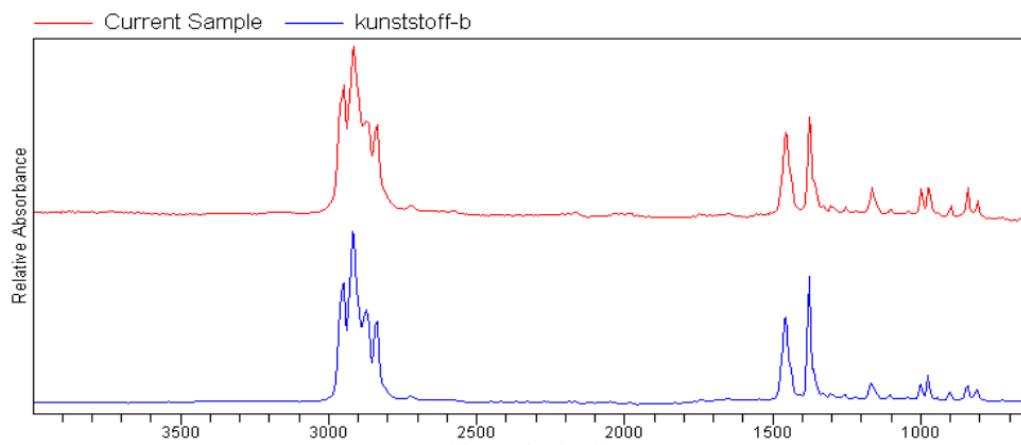


Figure 10: Sample 2 ATR-FTIR analysis

After the ATR-FTIR was done measuring the sample, it plotted an absorbance graph seen in Figure 10. It shows one narrow peak at around  $2900\text{ cm}^{-1}$ . This peak is an Alkane.

Additionally, there is a cluster in the lower region at around  $1400\text{ cm}^{-1}$  which matches a Hydrocarbons and Esters. The full list of data is shown in Table 3.

The blue graph matches the red graph neatly. The reference library suggested the sample is polyethylene.

Table 3: Sample 2 results

Peak [ $\text{cm}^{-1}$ ]	Functional groups	Possible compound
2910	$\text{CH}_3$ Valenz.	Alkane
1450	$\text{CH}_3$ and $\text{CH}_2$ deform.	Hydrocarbons/ Esters
1380	$\text{CH}_3$ Deform.	Hydrocarbons

### 3.3.3 Sample 3: Outside of a Twix bar wrapper

Sample 3 is a Twix bar wrapper found beside the railway in Horw.



Figure 11: Collection of Sample 3

The outside of the twix wrapper has a golden glossy texture and a red logo. The material is quite sturdy.

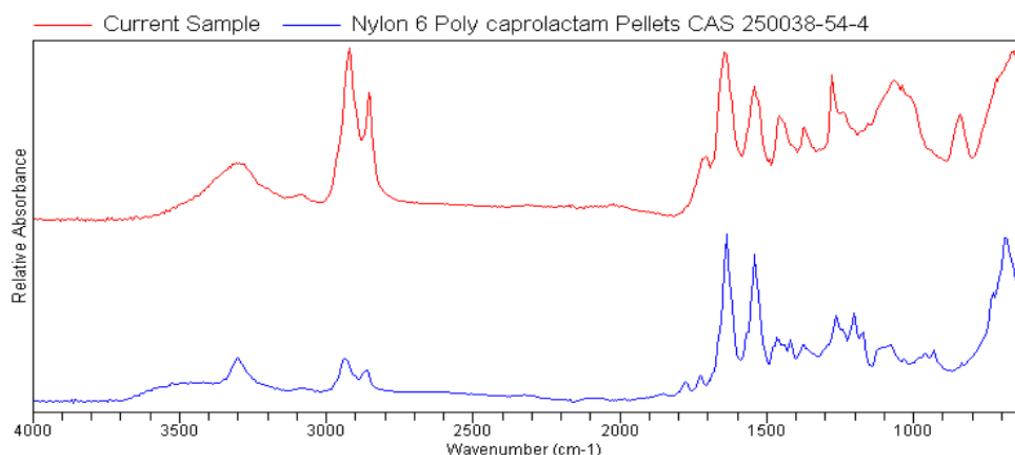


Figure 12: Sample 3 ATR-FTIR analysis

After the ATR-FTIR was done measuring the sample, it plotted an absorbance graph seen in Figure 12. It shows one broad band at around  $3300\text{ cm}^{-1}$ . The functional group is Amine/Amide.

Whats more, there is a massive peak at the frequency of approximately  $2900\text{ cm}^{-1}$ , very likely an Alkane. Followed by a big cluster of individual peaks from  $1700\text{ cm}^{-1}$  and downwards. The two major peaks correspond to Primary carbon acid amide and Nitroalkane. The full list of data is shown in Table 4.

The blue graph matches the red graph pretty decently but not perfect. The reference library suggested the sample is Nylon 6.

Table 4: Sample 3 results

Peak [ $\text{cm}^{-1}$ ]	Functional groups	Possible compound
3300 (broad)	N — H Valenz.	Amine/Amide
2940	$\text{CH}_3$ Valenz.	Alkane
1630	$\text{C}=\text{O}$ Valenz.	Primary carbon acid amide
1550	$\text{NO}_2$ Valenz.	Nitroalkane

## 4 Discussion

This section evaluates litter analysis in Horw and examines the results obtained from the Soxhlet extraction and ATR-FTIR measurements.

### 4.1 Litter in Horw

During the excursion, a survey was conducted in which trash samples were collected across the region of Horw in Luzern, spanning the area from the HSLU Campus down to Lake Lucerne.



Figure 13: Samples locations

In total, 17 different samples were collected, and their respective images can be found in subsection A.1. Out of the 17 trash samples collected, the Twix wrapper and the white foam were chosen as they were found next to the shoreline of the lake, where their potential environmental impact is greatest. The location of these samples can be seen in Figure 13 under the points 12 and 13, next to the Seerosenplatz.

This amount of litter collected is relatively little, which can be attributed to a couple of reasons. These include the availability of bins, regular cleaning and maintenance by the Horw municipality (Gemeinde Horw, 2025), and a culture that promotes responsible public behavior and environmental awareness (Binder & Hansmann, 2020a).

#### 4.1.1 Questions

The excursion required providing responses to seven questions related to litter and environmental conditions in Horw:

- Why might there be little to no litter in this area?
- What does this say about local waste management and environmental awareness?
- What might happen to this ecosystem if more people started visiting every day?
- What are potential hidden pollutants (microplastics, chemical runoff, etc.) even if no visible litter is present?
- How could community behavior or infrastructure (bins, signage, etc.) influence cleanliness?
- How could environmental education maintain or improve this standard?
- Record observations about waste bins, signage, or evidence of maintenance and report findings. How many waste bins did you see from HSLU until the lake?

The following points address the seven questions collectively.

#### 4.1.2 Availability of bins

In total, around 50 private bins and 15 public bins were seen on the route from HSLU to the lake. This means that people looking for a place to dispose of trash do not have to walk far to find a bin. Additionally, these bins were never overflowing, indicating that the Horw municipality empties them regularly. These factors encourage people to correctly dispose of their litter instead of throwing it onto the ground.

#### 4.1.3 Regular cleaning and maintenance

The fact that none of the bins were overflowing, and that regular road cleaning is carried out, indicates that the Horw municipality takes responsibility for local waste management and demonstrates high environmental awareness. Additionally, the municipality of Horw states that they are responsible for duties including: the operation and maintenance of streets, paths and public squares; the upkeep of green spaces, public playgrounds, and bathing/rest areas; the cleaning and maintenance of waste-collection points; and the daily emptying of public litter bins (Gemeinde Horw, 2025).

However, an increase in the number of daily visitors would lead to more littering and greater pollution, if strict waste disposal and education measures are not maintained. This can increase the workload on the municipality and have negative impacts on the ecosystem. For instance, litter along the lake shores can degrade the habitat quality and enter the food chain of the local wildlife.

#### 4.1.4 Public culture

In general, the Swiss culture encourages proper disposal of litter. A study in 2020 surveying 1206 participants across Switzerland found that Swiss residents generally have high environmental awareness and hold themselves responsible for environmental consequences. Additionally, some of the most frequently performed behaviors to combat environmental pollution consisted of avoiding littering and correctly sorting waste for recycling (Binder & Hansmann, 2020b).

This could be further improved by introducing environmental education including, but not limited to, workshops, school programs, and local awareness campaigns to emphasize the importance of proper waste disposal and appreciation of the lake ecosystem. Additionally, properly placed bins, clear signage, and community involvement in maintaining a clean neighborhood can help promote cleanliness.

#### 4.1.5 Invisible trash

Despite the absence of visible trash, many invisible elements still contribute to dangerous pollution and need to be taken into consideration. One of the major concerns is microplastics, which comprise plastic particles smaller than five millimetres and often barely visible. A study conducted by the Swiss Federal Institute of Aquatic Science and Technology, Eawag found that freshwater snails that ingested nanoplastics with their food were unable to reproduce (Carles et al., 2022). This is concerning due to the presence of the lake ecosystem nearby. Chemical runoff, detergents, fertilizers, or sediments along the lake are other concerns. These pollutants can accumulate over time in the ecosystem and in wildlife.

## 4.2 Soxhlet extraction: results interpretation

After the experiment for the decision of the solvent, ethanol was chosen due to its capability of removing rhodamine B effectively from the polystyrene sample without dissolving or damaging the plastic matrix. Ethanol is a polar alcohol molecule, leading to the conclusion that the dye is also partly polar. The polystyrene, which is a non-polar polymer, was not dissolved in the solvent. In contrast, diethyl ether and acetone caused the polymer to swell or soften, indicating partial solubility, but failed to extract the dye. Hexane, a strongly non-polar molecule, dissolved neither the matrix nor the dye.

With the change in color of the solvent and the matrix after the first extraction cycle in the Soxhlet experiment, the efficiency of the solvent with respect to the dye was demonstrated. Due to the low viscosity of the ethanol while boiling, the interaction with the matrix and the rhodamine B was enhanced, lowering consequently the cycle time.

### 4.2.1 Questions

1. Why does operating at the solvent's boiling point almost always improve extraction efficiency?

R: The boiling temperature enhances mass transfer due to the increased solubility of the solute and the decreased viscosity and surface tension of the solvent. The solvent interacts more effectively with the matrix because of the reduced thickness of the boundary layer. Soxhlet continuous reflux helps to renew the solvent and keep it warm, allowing for a faster and more complete extraction (Apyari et al., 2024).

2. In what ways can Soxhlet extraction reduce fresh solvent consumption compared with repeated batch extractions?

R: In Soxhlet extraction, the same portion of the solvent continuously boils and condenses, removing the necessity of replacing the solvent after each extraction phase, as required in repeated batch extraction. Moreover, the solvent in the thimble is automatically and continuously replenished, ensuring that it never becomes fully saturated.

3. Which other characteristics of rhodamine can help us with its identification?

R: Rhodamine B can be identified by its pink-purple color and by its strong fluorescence, and is easily excited under UV light.

4. What makes a solvent good for extraction?

R: The polarity of the solute plays a key role in selecting the most suitable solvent, as the solvent's polarity should match the solute's ("like dissolves like"). In organic extractions, the nature of the phytochemical constituents (bioactive compounds naturally present in plants) is also important. Moreover, the thermal stability and boiling point of the solvent are essential properties to consider (Lin et al., 2018).

## 4.3 ATR-FTIR analysis: results interpretation

This section provides an interpretation of the ATR-FTIR results, outlining the methodology used, the material identification process, and the environmental implications of the findings.

### 4.3.1 Questions

For the ATR-FTIR analyses, the following questions were asked:

- What is the purpose of using ATR-FTIR in environmental analysis?
- What does the absorbance spectrum represent?
- Compare your measured spectrum with reference spectra from the library what materials were identified?
- Discuss the environmental implications of finding plastics at the lake shore.
- How could the presence of these materials impact ecosystem health and aquatic life?

The following points address the seven questions collectively.

### 4.3.2 Methodology

To make a risk assessment of an environmental sample, the material must first be determined. Further analysis can then be conducted. ATR-FTIR is an excellent choice for two main reasons: it is portable for field use, and it is relatively inexpensive and reliable.

As explained in section 1, the ATR-FTIR uses an infrared beam, a crystal, and a detector, to generate an absorbance graph of the sample tested. The spectrum shows which frequencies of infrared radiation are absorbed by the material and to what extent. It can contain broad bands or sharp peaks. This pattern serves as a fingerprint to identify the material.

### 4.3.3 Identification

After each sample is measured, the computer automatically determines the best match for the resulting absorbance spectrum. However, this match can be incorrect, so it is essential to check and verify whether the peaks correspond accurately to the sample. The data presented in section 3 are now evaluated to determine the best-fitting material for each of the two samples.

#### Sample 1: White foam

Polyethylene, this is very plausible, due to it matching the measured graph nearly perfectly. Each frequency lines up exactly, and the magnitude of the peak is spot on. This result can be trusted.

#### Sample 2: Inside of a Twix bar wrapper

Polyethylene, this is also a very good match: all the frequency peaks, and magnitudes match. This result can be trusted.

#### Sample 3: Outside of a Twix bar wrapper

Nylon 6 Poly(caprolactam) Pellets, here it is harder to justify a 100% match, the frequencies match almost perfectly, but in the high-frequency region the magnitudes are very different. In the low-frequency region, some minor differences can be seen. All in all, this should still be a match, but caution is still advised.

### 4.3.4 Impact on the environment

Polyethylene is very stable and can persist in the environment for long periods. As a result, it can disperse far beyond its initial point of deposition. This process is accelerated by the fragmentation of the material into smaller pieces (Jang et al., 2022).

These smaller pieces, called microplastics, can remain in the environment for many years. They cause a range of harmful effects, many of which are still unknown. One significant effect is bioaccumulation (Adolphi et al., 2025), where microplastics are ingested by organisms, accumulate in their tissues, and are subsequently transferred up the food chain. In humans, this may increase the risk of cardiovascular diseases (Adolphi et al., 2025). In aquatic ecosystems, such as those in Lake Lucerne that contain fish and plants, this poses a significant risk to reproduction and long-term growth.

Nylon microplastics can also have a devastating impact on marine life. The feeding of primary and secondary producers may be impaired by the presence of microplastics. If these populations decline, a ripple effect could destabilize the entire food chain, resulting in reduced total biomass and diminished overall ecosystem health (Altin et al., 2019).

## 5 Conclusions

This study provided a two-part assessment of plastic waste in Horw: a field observation of litter prevalence and a chemical characterization of collected samples.

### 5.1 Field observation and Waste management

Walking along the road to the Lake Lucerne, marginal amounts of litter was found on the floor and around the lake. This can be attributed to few factors: the presence of numerous non-overflowing public bins, the culture around keeping Switzerland clean of waste, and the effective waste management by the Municipality of Horw. This effort helps preventing great amounts of trash entering the ecosystem and improves the stability of the local wildlife.

### 5.2 Characterization of waste

Despite the low quantity of litter in the environment, not all danger is averted. To prevent serious damage to the environment, compounds and additives must be determined to evaluate their potential hazard if they leach out into the soil, the water or the air.

To do this, ATR-FTIR samples analysis were performed. The material was identified as Polyethylene (PE), low-density Polyethylene (LDPE), and Nylon 6. The presence of these materials is a known environmental hazard, as they persist for long durations and degrade into microplastics, which harms local wildlife and ecosystems.

### 5.3 Methodological assessment and Future work

The experiment validated the potential of the Soxhlet extraction as a complementary analytical tool. A proof-of-concept experiment using rhodamine B dye confirmed the method's effectiveness in separating additives from a polymer matrix.

Future work should now apply the Soxhlet extraction method to the collected trash samples, allowing for the isolation and identification of the specific additives within the Polyethylene and Nylon 6. The study of waste is critical for assessing the potential risks to the water and soil systems around Lake Lucerne.

## A Appendix

### A.1 Inventory of samples collected

The following section contains images and GPS coordinates of the 17 samples collected during the excursion. The coordinates are in CH1903+ / LV95 format.

1. Wrapper 1



2'665'899.47, 1'207'031.49  
(Altitude: 441 m)

2. Wrapper 2



2'665'901.72, 1'207'034.36  
(Altitude: 442 m)

3. Cigarette



2'665'912.30, 1'207'003.50  
(Altitude: 440 m)

4. White plastic piece



2'665'936.06, 1'206'975.89  
(Altitude: 438 m)

5. AA battery



2'665'914.68, 1'206'981.87  
(Altitude: 439 m)

6. Zip tie



2'665'970.32, 1'206'911.43  
(Altitude: 436 m)

7. Liquid protein wrapper



2'665'944.39, 1'206'793.80  
(Altitude: 435 m)

8. Black plastic piece



2'665'946.13, 1'206'700.62  
(Altitude: 436 m)

9. Metal bottle cap



2'665'930.13, 1'206'552.52  
(Altitude: 434 m)

10. Aluminum can 1



2'665'924.26, 1'206'512.29  
(Altitude: 434 m)

11. Wrapper 3



2'665'921.52, 1'206'555.81  
(Altitude: 436 m)

12. Twix wrapper



2'665'921.52, 1'206'555.81  
(Altitude: 436 m)

13. White foam



2'665'917.63, 1'206'549.37  
(Altitude: 437 m)

14. Wrapper 4



15. Evliya wrapper



2'665'996.78, 1'207'103.27  
(Altitude: 438 m)

16. Aluminum can 2



2'665'995.95, 1'207'102.94  
(Altitude: 438 m)

17. Plastic bottle cap



2'665'956.94, 1'207'223.33  
(Altitude: 442 m)

## A.2 ATR-FTIR analysis

Table 5: Infrared absorption bands for Functional groups identification

Wavenumber (cm <sup>-1</sup> )	Vibration	Compounds
3700–3600	O–H stretching	Alcohols, phenols, acids
3500–3300	O–H stretching (broad)	Alcohols, phenols, acids
3550–3350	N–H stretching (unassociated)	Primary/secondary amines, amides
3500–3100	N–H stretching (associated)	Primary/secondary amines, amides
3300–3270	≡C–H stretching	Monosubstituted alkynes
3350–3150	NH <sub>3</sub> <sup>+</sup> stretching (broad)	Aminohydrochlorides
3300–2500	O–H stretching (very broad)	Carboxylic acids
3100–3000	=C–H stretching	Aromatics, alkenes
3000–2800	C–H stretching	Alkanes, cycloalkanes
2962, 2872	CH <sub>3</sub> stretching	Alkanes
2926, 2853	CH <sub>2</sub> stretching	Alkanes
2820	CH <sub>3</sub> stretching	Methyl ethers
2300–2100	C≡X stretching (X = C, N, O)	Alkynes, nitriles
2190–2100	C≡C stretching	1,2-disubstituted alkynes
2245–2220	C≡N stretching	Nitriles
2140–1970	C≡C stretching	Monosubstituted alkynes
1900–1660	C=O stretching	Carbonyl compounds
1850–1800	C=O stretching	Acid halides
1840–1780	C=O stretching	Acid anhydrides (2 bands)
1780–1650	C=O stretching	Saturated carboxylic acids
1760–1700	C=O stretching	Saturated esters
1740–1710	C=O stretching	Aldehydes/ketones; $\alpha, \beta$ -unsaturated and aromatic esters
1745	C=O stretching	Cyclopentanone
1715	C=O stretching	Cyclohexanone
1715–1680	C=O stretching	$\alpha, \beta$ -unsaturated and aromatic aldehydes
1690–1660	C=O stretching	$\alpha, \beta$ -unsaturated and aromatic ketones
1680–1630	C=O stretching	Primary amides (Amide I)
1660–1600	C=C stretching	Aromatics, alkenes
1650–1620	NH <sub>2</sub> deformation	Primary amides (Amide II)

Wavenumber (cm <sup>-1</sup> )	Vibration	Compounds
1650–1580	N–H deformation	Primary and secondary amines
1630–1615	H–O–H deformation	Crystalline water
1630–1590	Ring vibration	Aromatics
1560	NO <sub>2</sub> stretching	Nitroalkanes
1520	NO <sub>2</sub> stretching	Aromatic nitro compounds
1518	—	Aromatic nitro compounds
1500–1480	Ring vibration	Aromatics
1480–1430	CH <sub>3</sub> , CH <sub>2</sub> deformation	Hydrocarbons, esters
1420–1340	O–H deformation	Alcohols, phenols, carboxylic acids
1390–1370	CH <sub>3</sub> deformation	Hydrocarbons
1360–1030	C–N stretching	Amides, amines
1350–1420	NO <sub>2</sub> stretching	Aliphatic and aromatic nitro compounds
1290–1050	C–O stretching	Ethers, alcohols
1250–1180	C–O stretching	Saturated esters
1200–600	C–H deformation / ring	Alkanes, cycloalkanes, alkenes, substituted aromatics
970–960	C–H deformation	1,2-disubstituted alkenes (trans)
965–885	—	Monosubstituted alkenes
915–905	C–H deformation	1,3-disubstituted benzenes
830–750	—	—
815–750	C–H deformation	1,2-disubstituted aromatics
855–825	C–H deformation	1,4-disubstituted aromatics
770–735	C–H deformation	1,2-disubstituted benzenes
740–680	C–H deformation	Monosubstituted benzenes
710–690	—	Alkanes with >4 CH <sub>2</sub> groups
670–650	C–H deformation	1,2-disubstituted alkenes (cis)
690–610	C–H deformation	Benzene
620–490	C–I stretching	Aliphatics
700–500	C–Br stretching	Aliphatics

## List of Figures

1	Soxhlet extractor components . . . . .	3
2	Graphical representation of a single bounce ATR (Specac Ltd., 2024) . . . . .	3
3	Rhodamine B . . . . .	4
4	Measurement procedure for the sample “Twix inside” . . . . .	5
5	Measurement procedure for the sample “Twix outside” . . . . .	5
6	Result of the solvents effectiveness experiment . . . . .	6
7	Collection of Sample 1 . . . . .	7
8	Sample 1 ATR-FTIR analysis . . . . .	7
9	Sample 2 during the analysis . . . . .	8
10	Sample 2 ATR-FTIR analysis . . . . .	8
11	Collection of Sample 3 . . . . .	9
12	Sample 3 ATR-FTIR analysis . . . . .	9
13	Samples locations . . . . .	10

## List of Tables

1	Candidate solvents properties and effectiveness . . . . .	6
2	Sample 1 results . . . . .	7
3	Sample 2 results . . . . .	8
4	Sample 3 results . . . . .	9
5	Infrared absorption bands for Functional groups identification . . . . .	18

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## Declarations on the use of AI tools

- “*ChatGPT 5.1*” was used to enhance vocabulary.  
*All original sentences originate from our own ideas and were refined with the support of this tool.*  
<https://chatgpt.com/>
- “DeepL” was used as a spell-checker.  
<https://www.deepl.com>
- “Google Gemini” was used as a fact-checker.  
<https://gemini.google.com/app>