From practice: Edible oil as an atypical chemical trace

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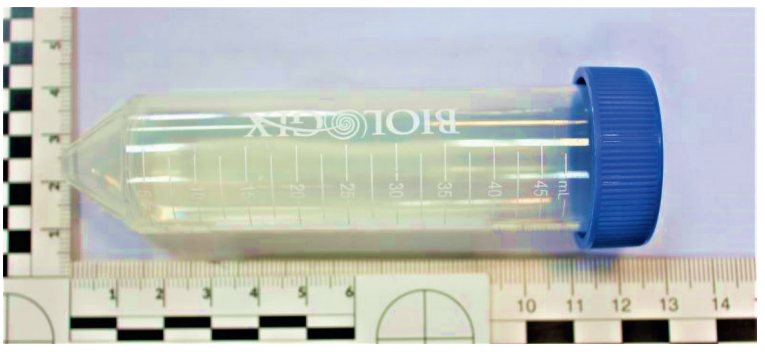
Abstract

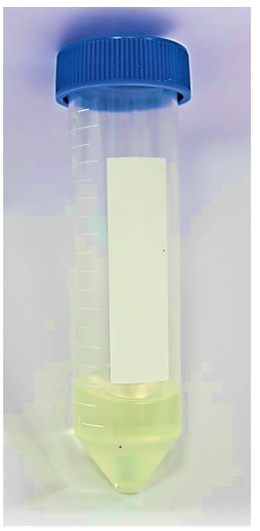
The article discusses a case solved as part of the implementation of a forensic opinion in the field of chemical tests. It presents the course of action with the evidence identified as nn. substance. In the article, the possibilities of drawing conclusions regarding properties and hazards based on publicly available Material Safety Data Sheets are presented.

Keywords: chemical research, nn. substances, FTIR (ATR), GC/MS

The term "unusual chemical traces", or the so-called nns, is used in laboratory practice to refer to material evidence that cannot be easily classified into a specific field, e.g. flammable substances, alcohols, narcotic drugs, microtraces or explosives.

The investigation regarding such traces should begin with a thorough analysis of the decision, contact with the person conducting the proceedings in order to clarify often general questions, but also analysis of inspection reports or illustrative material in the form of photographs of the packaging of the original traces.





Photograph 1–2. Method of securing the sent evidence

The remaining part of the article demonstrates the importance of collecting relevant information before starting the study.

For the study, a plastic test tube containing a light yellow oily substance was obtained (Photograph 1 and 2). The evidence was additionally placed in a paper envelope with a trace ID. The data sheet showed that the substance was taken from a 750 ml glass bottle with a sticker reading "THOMY".

The incident concerned water contamination by pouring an unknown liquid into a city water hydrant, i.e. an act under Art. 182 § 1 of the Penal Code.

The questions included in the decision to admit expert evidence were:

"1. Of what type is the light yellow oily substance sent for testing in a quantity of 10ml?

2. Is this substance a hazardous substance that poses a threat to human life or health?

3. Can this substance cause water pollution in such an amount and in such a way that it may threaten human life or health or cause a significant reduction in water quality?

Indeed, it can be assessed at the very beginning that the scope of the tests ordered by the decision exceeds the competences of an expert in the field of chemical tests. However, one should consider whether to refuse to perform identification tests for the evidence on the grounds that one cannot answer further questions. It is known from the expert's experience that a tested substance, described at the stage of securing as "anthrax", turns out to be baking soda, and the requested "corrosive substance" used to intimidate the victim – turns out to be table salt.

One of the important stages of study is the assessment of the trace, its form and determining the scope of study. In this case, telephone arrangements made with the person conducting the proceedings were important. It was established that the light yellow oily liquid in question was poured from a brown glass bottle with a label. After sending photographs of the labels to the expert (photograph 3 and 4), it turned out that the bottle, according to the label, contained sunflower oil with a high content of vitamin E and unsaturated fatty acids.

Photograph 3. The packaging from which the liquid sample was secured

Photograph 4. Packaging label

As part of the preliminary physicochemical tests, the characteristics of the substance were analysed to determine whether the transferred liquid could be vegetable fat (in accordance with the label – edible oil). The following was assessed:

- appearance and odour of the substance;
- whether it causes greasy stains on a piece of paper that fluoresce under ultraviolet light;
- the solubility of the sent liquid sample in water was checked – insoluble;
- pH tests – pH ~7 (neutral).

8 ml of light yellow oily liquid were used for further tests. At the same time, due to the type of the tested substance, reference substances (rs) were selected in the form of:

- sunflower oil – light yellow oily liquid;
- rapeseed oil – light yellow oily liquid;
- linseed oil – yellow oily liquid;
- castor oil – light yellow thick oily liquid;
- olive oil – yellow oily liquid.

Comparative studies of the chemical compositions of the sent liquid and the reference substances were performed using the Nicolet iS50 IR spectrometer from Thermo Scientific, using the attenuated total reflectance (ATR) technique.

As a result of the conducted testing, spectra were obtained (Fig. 1–4), based on the analysis of which it was concluded that:

- the chemical composition of the sent liquid sample is similar to the chemical composition of sunflower oil;
- the chemical composition of the sent liquid sample differs slightly from the chemical composition of rapeseed oil;
- the chemical composition of the sent liquid sample differs from the chemical composition of castor oil, linseed oil and olive oil.

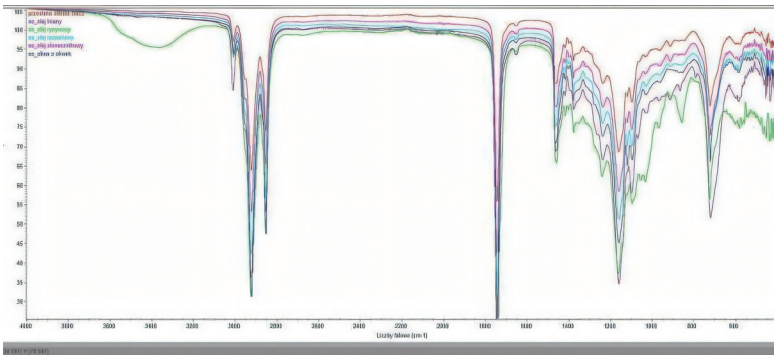


Fig. 1. Summary of infrared spectra of the test substance and all reference substances

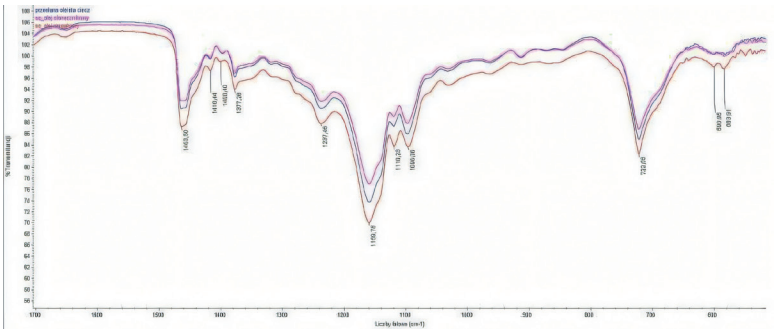


Fig. 2. Summary of infrared spectra of the test substance and similar reference substances with significant spectral ranges marked

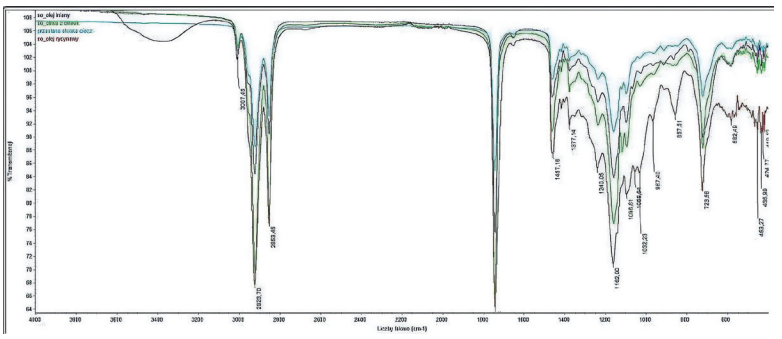


Fig. 3. Compilation of infrared spectra of the test substance and different reference substances

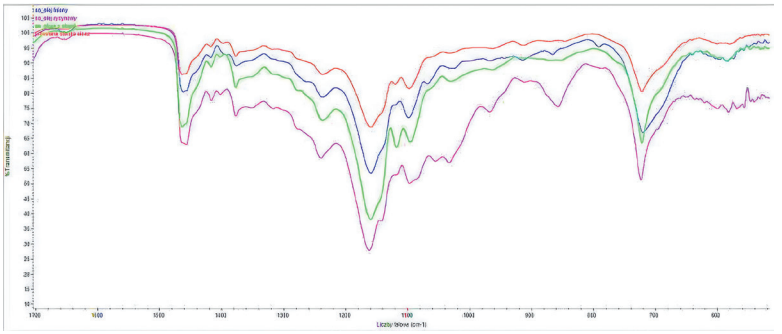


Fig. 4. A compilation of infrared spectra of the test substance and different reference substances with significant spectral ranges marked

In order to determine the presence of unsaturated fatty acids, samples of the sent liquid and sunflower and rapeseed oil were treated with a 10% solution of KOH in MeOH. After heating the mixture, toluene and water were added. After phase separation, the upper organic part of the liquid was collected. This operation, called transesterification, enables GC analysis of fatty acids contained in glycerides in the form of their methyl esters.

Additionally, part of the sample of the sent liquid was extracted with methanol to examine other components of the sample, apart from fatty acids, e.g. vitamin E.

The extracts were analysed using a TraceGC 2000 gas chromatograph coupled with a PolarisQ mass spectrometer from Finnigan.

Based on the analysis of the obtained chromatograms and mass spectra (Fig. 5–7), the presence of a mixture of unsaturated fatty acids and vitamin E was found in the samples of the sent liquid.

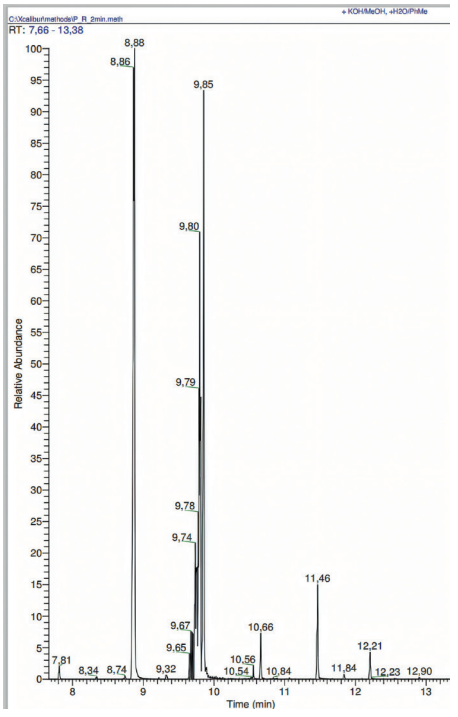


Fig. 5. Result of GC/MS analysis of the sent liquid after transesterification. Fatty acid residues in esters: C16:0 palmitic, C18:0 stearic, C18:1 oleic, C18:2 linoleic, C18:3 linolenoic, C20:4 arachidonic, C20:5 eicosapenteanoic, C22:6 docosahexaenoic

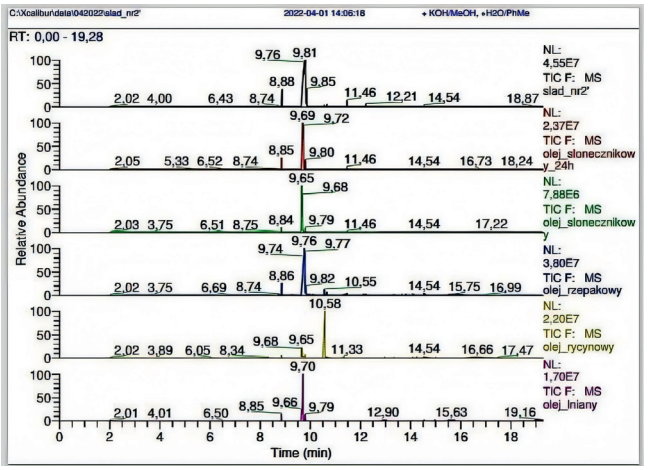


Fig. 6. Comparison of the chemical compositions of the transferred liquid and the reference substance after transesterification

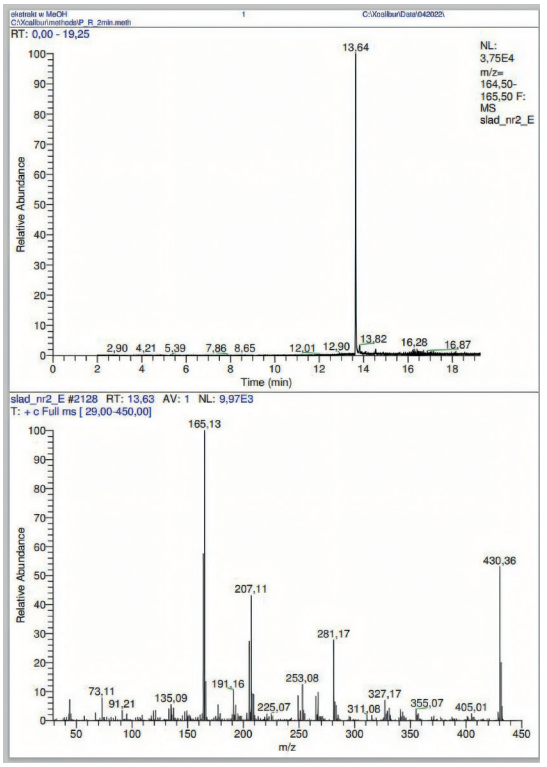


Fig. 7. Ion current chromatogram m/z = 165 and mass spectrum of vitamin E.

Summarizing the tests performed, it can be stated that the tested sample of the substance in its appearance and consistency (light yellow oily liquid) corresponds to the reference substances in the form of sunflower or rapeseed oil. Its chemical composition is similar to the oil types mentioned above. It also contains vitamin E, which (according to the information contained on the label of the bottle from which the liquid sample was taken) is present in sunflower oil by Thomy

In the opinion, based on the study conducted, the following conclusions are made:

1. The physical characteristics and chemical composition of the light yellow oily substance sent for testing indicate that it is vegetable oil containing vitamin E. This is consistent with the data contained on the label of the bottle from which the liquid sample was secured;
2. According to the sample Safety Data Sheet for edible sunflower oil attached to the opinion, the substance is non-toxic and biodegrades when released into the environment (soil). Additionally, the Safety Data Sheet contains information that the product should not be poured into sewers or sewage. Do not pour into water or sewage systems. Apply general principles of waste management.

Despite the lack of reference to toxicology, it was possible, thanks to publicly available Material Safety Data Sheets, to answer most of the questions included in the decision. What is important in this case is that the perpetrator of the act polluted the water.

Edible oils are not single-component substances. These are mixtures of triglycerides and additives such as vitamins. Edible fats become rancid due to the oxidation of unsaturated acids under the influence of air, resulting in the formation of aldehyde compounds. Rancidity of butter, margarine and oil is also caused by the process of hydrolysis (in the presence of water), which leads to the formation of free fatty acids. This impairs the properties of edible oils and creates an unpleasant odour and aftertaste, which may significantly reduce the quality of drinking water in municipal hydrants.

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