Chemical forensics

March 2024

For more information, contact us:

Sarah Clapham
Science Policy Officer
sarah.clapham@opcw.org

Peter Hotchkiss
Science Policy Adviser
peter.hotchkiss@opcw.org

Contents

1

Definitions

Forensic science

Forensic science is the application of scientific methods and techniques to examine evidence for investigative purposes, usually relating to legal matters. These methods and techniques are drawn from diverse scientific fields, such as biology, physics, and chemistry. Common forensic tools include DNA sequencing, fingerprinting, high-speed ballistics photography, and drug testing.

Chemical forensics

Chemical forensics is the application of analytical chemistry methods and techniques to examine evidence (chemical traces) for investigative purposes. The goal of chemical forensics is to leverage distinctive signatures, such as known impurities and byproducts, to obtain additional information on how and where a particular chemical was produced or originated.

Chemical forensics – key terms

Profiling: analysis of the chemical composition of a substance to create a profile or characteristic pattern. This typically includes identifying and quantifying the various chemical constituents present in a sample.

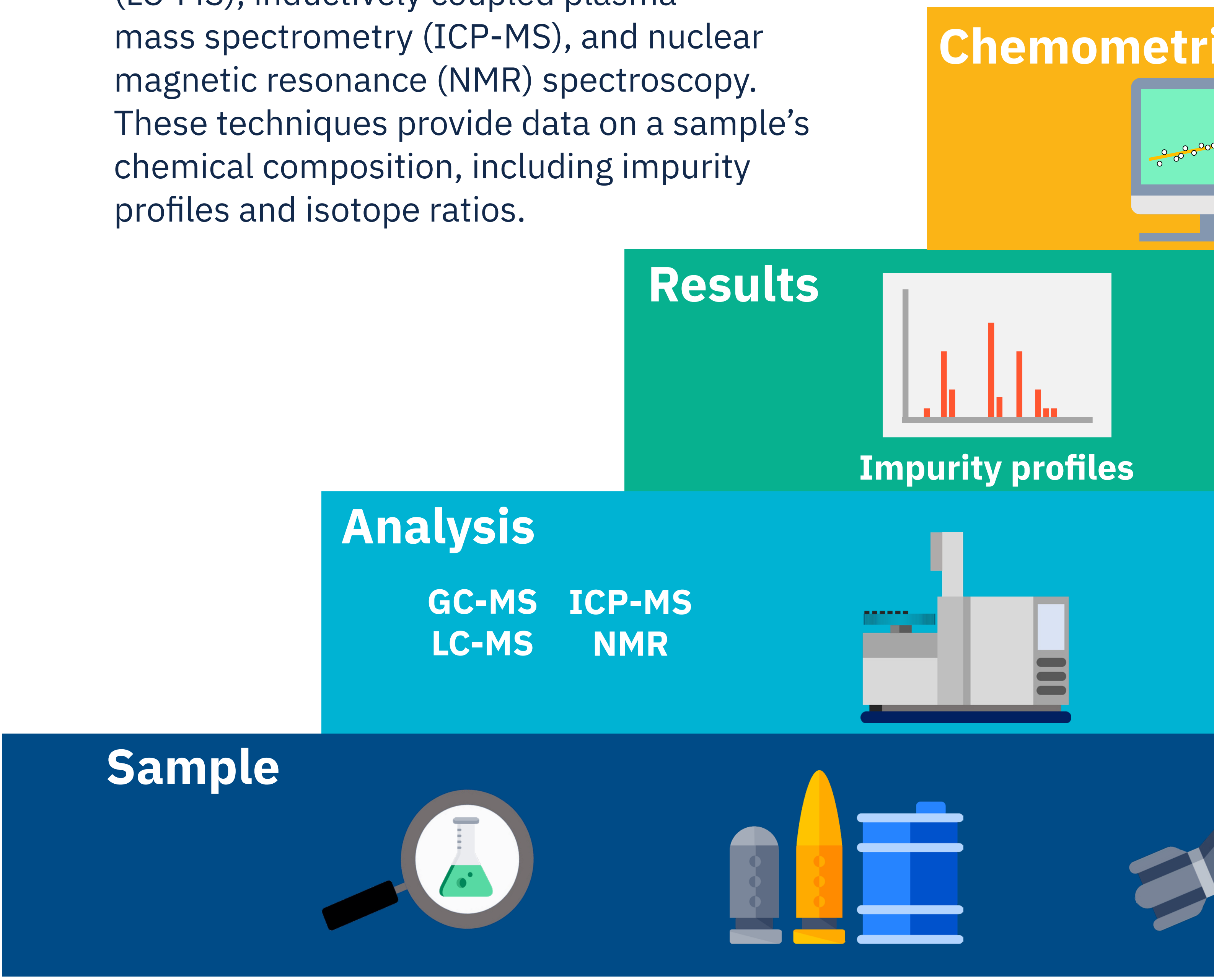
Fingerprint: a unique or characteristic pattern of chemical compounds present in a substance. Chemical fingerprints, like human fingerprints, can be used for identification purposes.

Signature: a set of specific markers or characteristics associated with a particular source, process, or condition which allow samples of a substance to be distinguished.

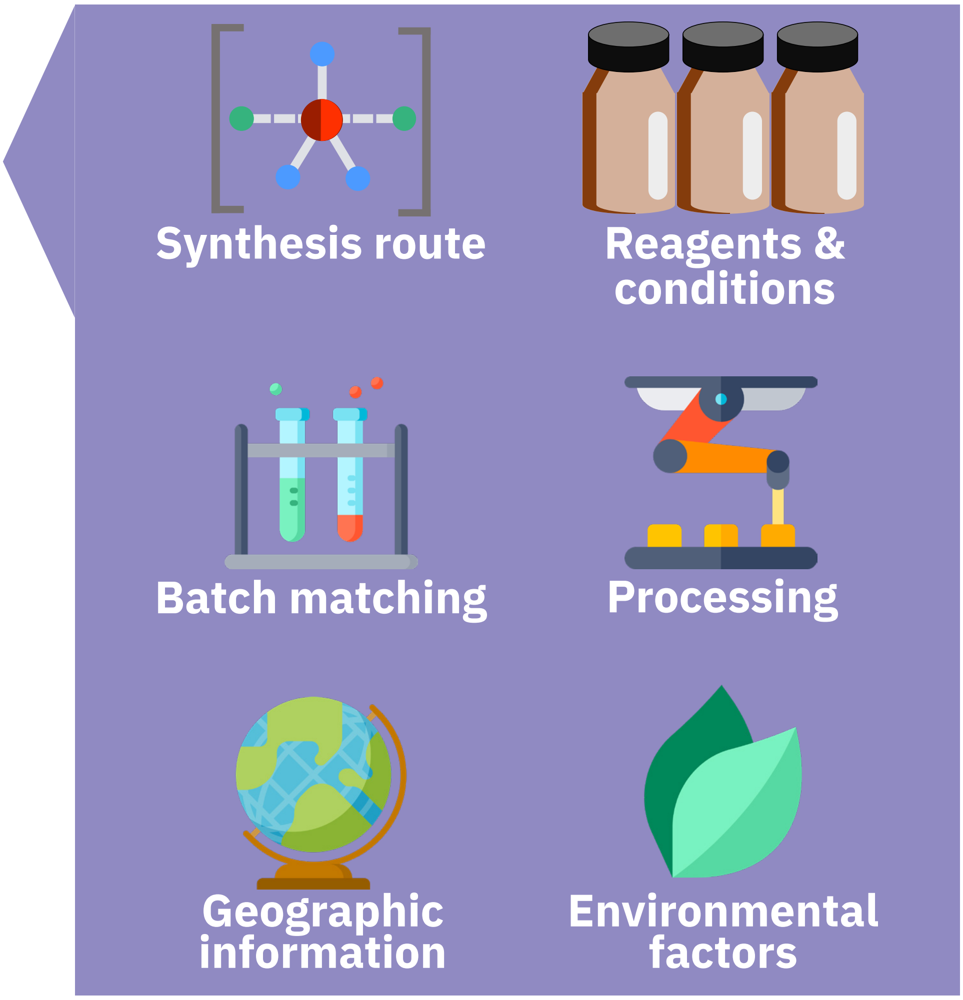
Provenance: the chronology of ownership, custody and/or location of a substance, including its production, distribution, and any changes it may have undergone.

Overview of chemica

Chemical samples from investigations can be information-rich sources of evidence. They are analysed using various techniques, such as gas chromatography-mass spectrometry (GC-MS), liquid chromatography-mass spectrometry (LC-MS), inductively coupled plasma-mass spectrometry (ICP-MS), and nuclear magnetic resonance (NMR) spectroscopy. These techniques provide data on a sample’s chemical composition, including impurity profiles and isotope ratios.



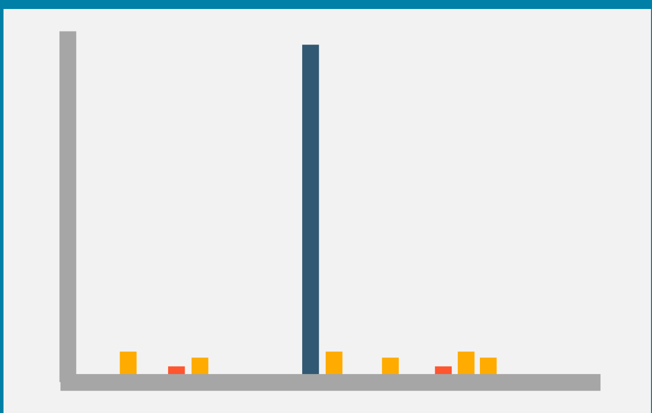
l forensics



A wealth of information on the sample can then be extracted from these data using chemometrics. This is an area of chemistry that uses mathematical and statistical approaches to extract information from chemical data. It can be used to identify patterns and make predictions about chemical systems. This is highly pertinent to investigations into the use of chemical weapons as it can provide vital information.

Impurity profiles

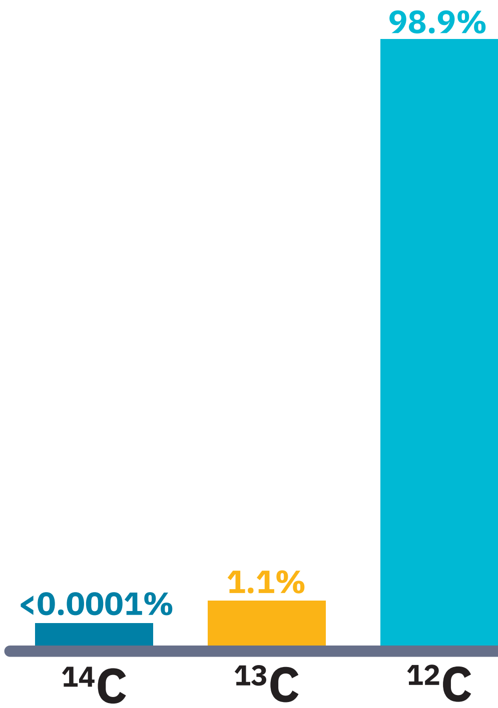
No chemical compound is 100% pure; in other words, it always contains traces – often in minute quantities – of other chemical species. These traces are known as impurities, and examples include residual solvents, catalysts, unreacted precursors, byproducts, manufacturing contaminants, and degradation products. Analysis of impurities in chemical compounds can provide unique impurity profiles that can be used as forensic signatures.



Isotope

Let's first briefly

Many chemical elements e
forms, known as isotopes.
different forms (isotopes)
called "carbon" and react
differences in their physic
chemical compound with c
carbon isotopes.



Impurity profiles and isoto
gain insights into the prod
findings.

ratios

explain whan an isotope actually is.

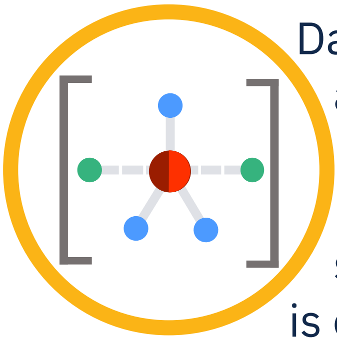
exist in two or more slightly different . For example, there are three slightly of carbon atoms. They are all still the same way but have very subtle al properties (e.g., their mass). Any carbon atoms will contain all three

You may have heard of carbon dating which is used to determine the age of materials, such as fossils and trees, that originated from living organisms. In this process, the amount of carbon-14 (a carbon isotope) is measured.

The different amounts of the three isotopes of carbon in a chemical compound can be measured, giving an isotope ratio. This ratio can be determined for any element that has isotopes. A number of factors (such as geographic location, environmental changes, and chemical synthesis) may affect the ratio of isotopes present in a given element. Isotope analysis can provide additional information about chemical compounds and, notably, may be used to discriminate between compounds that are indistinguishable by other analytical techniques.

ope ratios may be leveraged, either independently or collectively, to uction history, precursors, and processing methods, and corroborate

Information



Data from analytical results, such as impurity profiles and isotope ratios, can be used to determine additional information relating to the production history of a chemical. It is possible to establish how a substance was produced (its synthesis route), which is especially important when a single chemical can often be produced in many different ways. There are more than 10 different ways to produce sulfur mustard, for example!

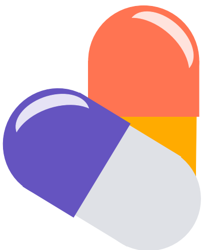
Analytical data can also identify the chemicals used (reagents), reaction conditions, and details about post-synthesis processing (e.g., purification) that may have taken place. Information on precursors and even the manufacturer can be inferred.

Chemicals may undergo specific reactions when exposed to environmental factors such as heat, cold, or humidity. Identifying markers for these changes could help identify a potential transport route, storage conditions, or even a season when the chemical was produced.

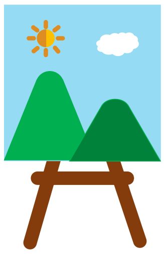
Chemical forensics techniques can also provide useful geographic information. For example, chemicals produced in a specific geographic region may have a different isotopic signature to those from other regions. Furthermore, production routes identified may be region-specific.

Examples

There are diverse applications of chemical forensics techniques across various fields, including criminal investigations, environmental monitoring, food safety, and pharmaceutical analysis.

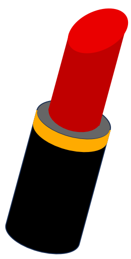


Chemical forensics techniques are an indispensable tool in illicit drugs investigations and in tracking clandestine drug manufacturing operations. Illicit drugs extracted from plants – such as cocaine or heroin – can present signatures or fingerprints inherited from the natural sources from which they are obtained. Minerals in the water used for irrigation or the altitude at which a plant was grown are examples of factors which cause identifiable changes in the plant's chemical composition. The identification and quantification of these marker chemicals enable the provenance of an illicit drug to be determined. Impurities such as solvent residues, intermediates and byproducts all provide additional information about the drug's production method.



The age and geographic origin of the materials used in works of art can be determined by isotope ratio analysis to confirm that the artwork is not a forgery.

The authenticity of olive oil, and other foods, may be determined by analysing its chemical composition to verify its origin.



Determining the chemical composition of cosmetics identifies discrepancies and detects the presence of harmful ingredients such as lead and chromium.

GC-MS: separation by

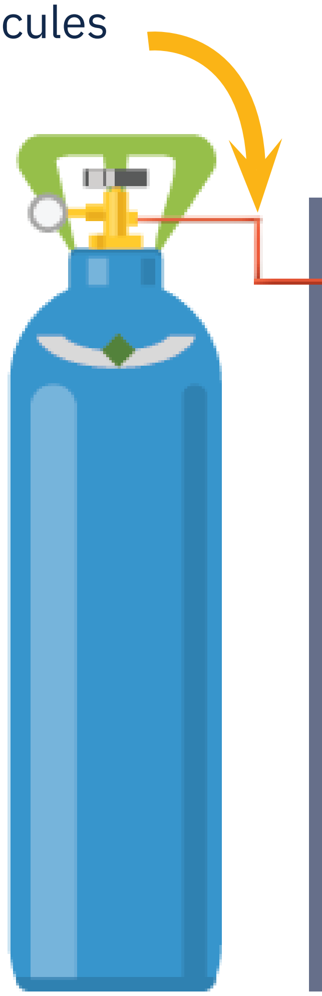
Imagine a relay race...

1 The athletes take their starting positions. The starting pistol is fired, and everyone sets off simultaneously.

2 As the race proceeds, differences in their ability emerge and the runners progress at different speeds, causing the starting pack to separate and spread out along the track. The further they run, the greater the distance between the runners.

3 The first group of runners approaches the second leg, where the next runners await them at the crossover box.

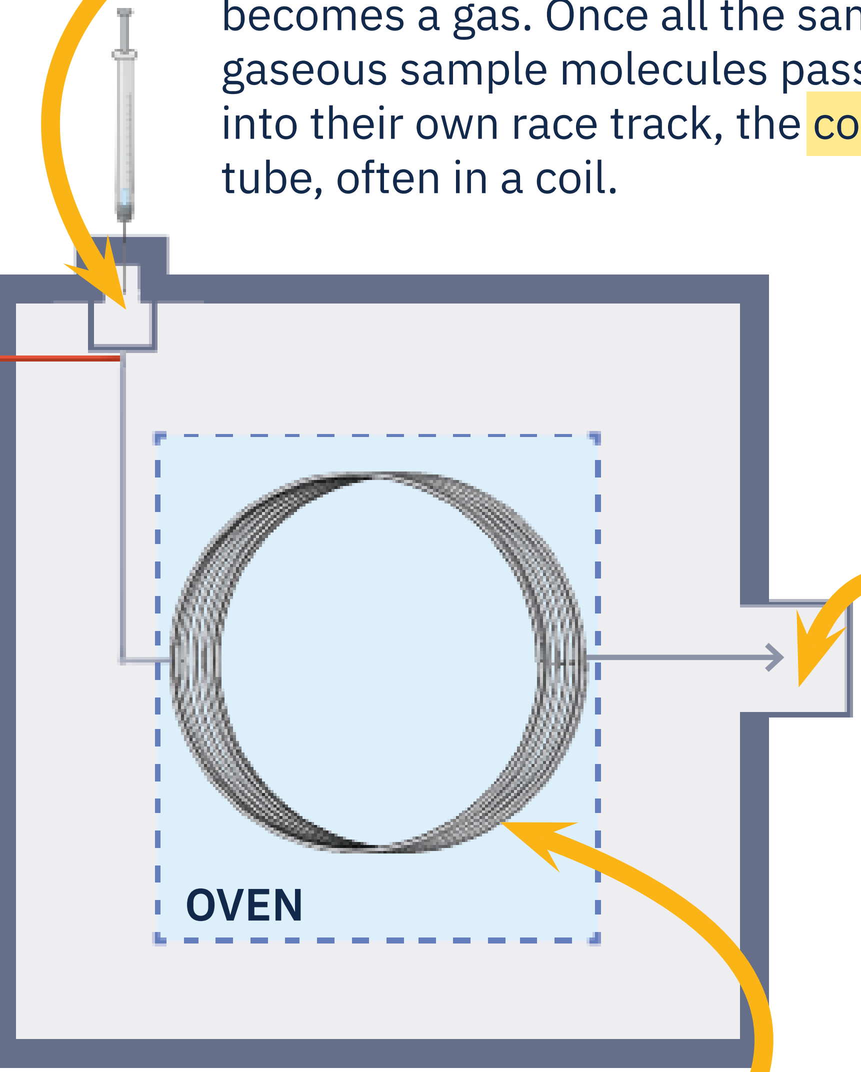
A carrier gas transports the sample gas molecules through the column.



2 Although the gas molecules sta
in their physical and chemical p
which they progress through the col
their speed, but molecules that are
molecular weight will pass through t

gas chromatography

1 The starting blocks for a gas chromatography (GC) instrument is the sample injection unit, where the liquid sample is injected. Just as the athletes warm up before the race, the liquid sample is warmed up until it becomes a gas. Once all the sample is vapourised, the gaseous sample molecules pass through the injection port into their own race track, the column – a very long, thin tube, often in a coil.



3 The separated gas molecules leave the GC and approach the interface (crossover box equivalent) with the mass spectrometer (MS).

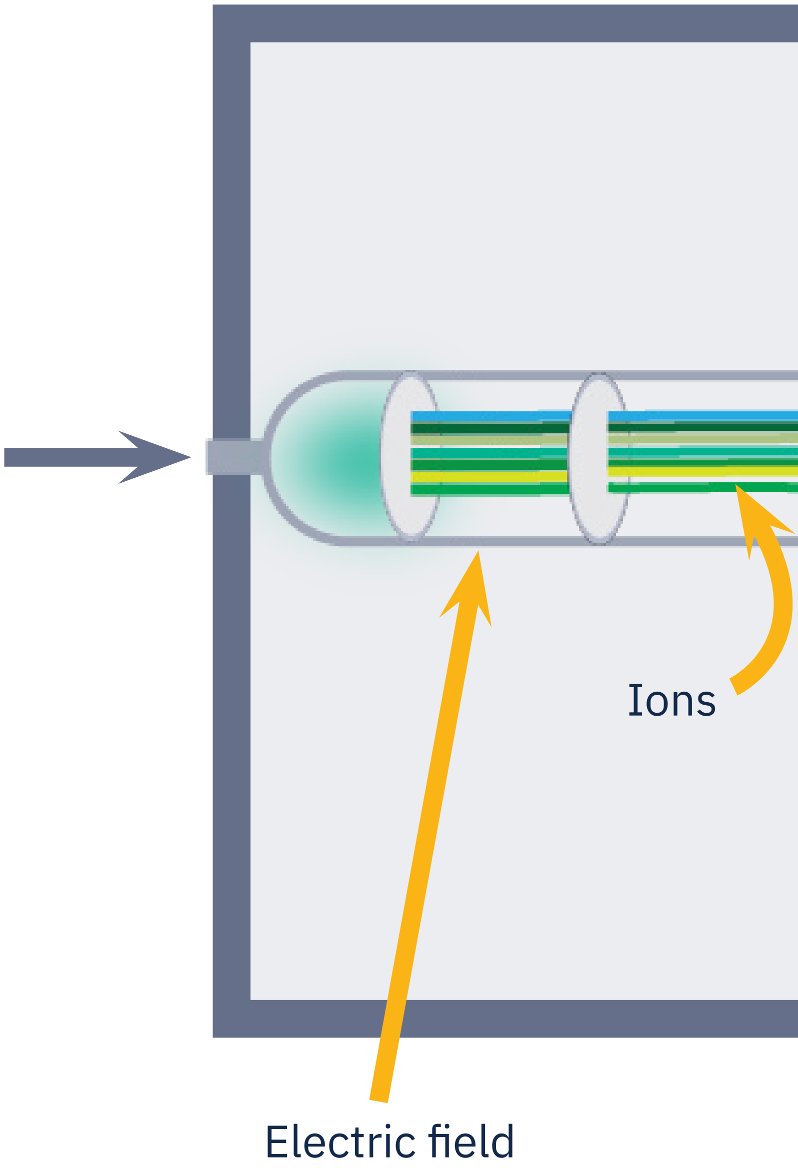
art their race together, differences
properties affect the speed with
lumn. A number of factors influence
highly volatile or have a low
the column the quickest.

GC-MS: identification

4 The baton is passed, and the second group starts. Fully energised, the second group accelerates away from the changeover box. The lines on the ground guide the runners around the curves in the track.

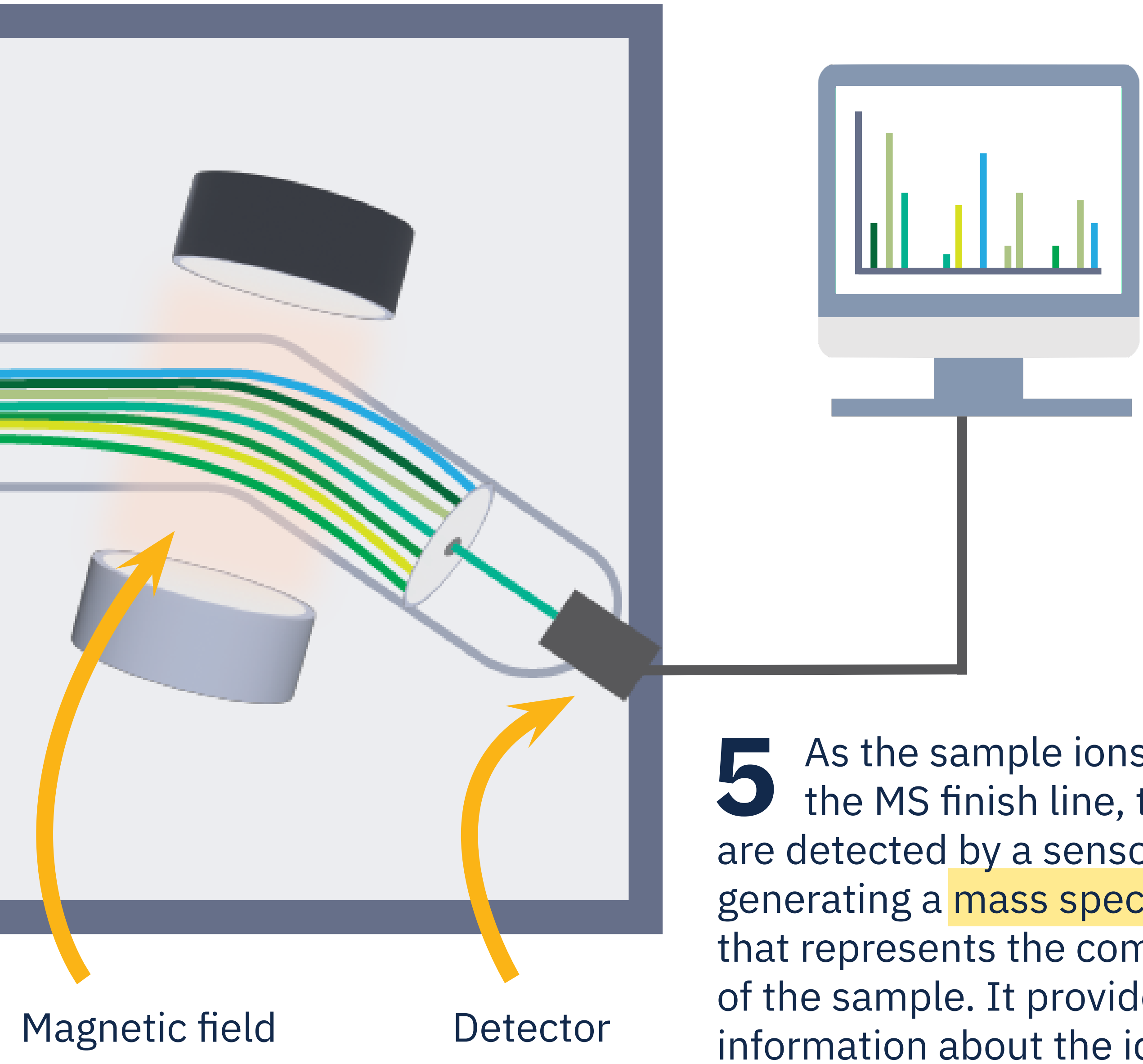
5 As the runners cross the finishing line, their chip timer records their race times generating a list of finish times for the leaderboard.

4 The uncharged sample molecul
into smaller fragments. An elect
depending on their mass, their path i



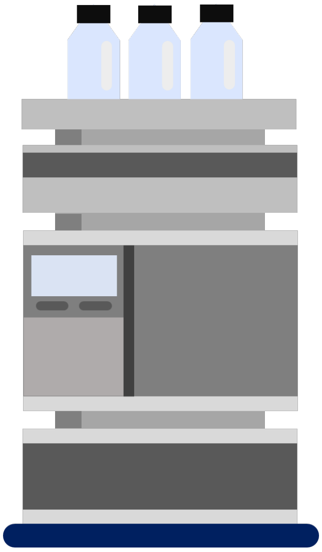
by mass spectrometry

es are transformed into charged particles – ions – which then break tric field causes them to accelerate through the mass analyser, and s deflected (curved) by a magnetic field.



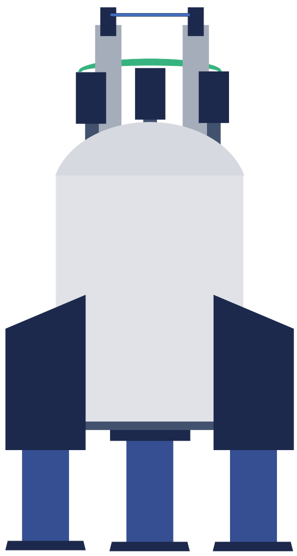
5 As the sample ions cross the MS finish line, they are detected by a sensor, generating a mass spectrum that represents the composition of the sample. It provides information about the identity and quantity of the compounds present in the sample.

Other techniques



Other chromatography-based techniques
High-performance liquid chromatography (HPLC) and LC-MS are two more versatile analytical techniques for the separation, identification, and quantification of complex mixtures of compounds. Compared to GC-MS, HPLC and LC-MS are better at analysing compounds that are thermally sensitive or substances which have areas of positive or negative charge, as they operate at lower temperatures and use a liquid solvent to transport the sample through the instrument.

Nuclear magnetic resonance spectroscopy
Just like the mass spectrometer component of GC-MS and LC-MS instruments, NMR spectroscopy also makes use of magnetic fields to extract information from a molecule about its structure. NMR spectroscopy is less sensitive than mass spectrometry-based techniques and so more sample is used in the analysis. However, unlike GC-MS and LC-MS, NMR spectroscopy is a non-destructive technique, meaning that the sample can be recovered after analysis. This is a very convenient feature in those cases where the sample is limited.



Opportunities

Increased deterrence: Exploitation of samples using chemical forensics tools can lead to identification of their source, a powerful deterrent against the use of chemical weapons.

Enhanced legal tools: The information afforded by chemical forensics tools is crucial to international organisations like the OPCW for the identification of perpetrators, ultimately strengthening any legal response by the responsible judicial authorities to chemical attacks.

Expanding chemical forensics capabilities: As technology advances, the scope and capabilities of chemical forensics continue to expand. For example, using artificial intelligence to search databases will increase speed and improve pattern recognition.

Limitations

Size and scope of chemical databases: the successful application of chemical forensics tools to analyse chemical weapons use requires comprehensive, international databases of chemical signatures. As things stand, limited databases and cooperation reduce the effectiveness of current chemical forensics techniques and efforts.

Validation and standardisation: Chemical forensics is an important element in the process of identifying perpetrators of chemical weapons use. However, a lack of internationally accepted standards and protocols, and validated methods means that full capability of the field cannot yet be leveraged.

15

TWG on chemical for

Chemical forensics is highly relevant to the work of the Organisation and its importance has been highlighted by the previous Temporary Working Groups (TWGs) on Investigative Science and Technology and Analysis of Biotoxins. There is growing concern around the misuse of chemicals, such as by non-State actors as well as more targeted use by States. It is more important than ever that as much information as possible be derived from samples from an alleged attack. Thus, it is imperative that the OPCW be able to fully understand and harness the utility of chemical forensics approaches and be able to use validated results in any investigation of misuse of a chemical. A deeper understanding of chemical forensics is also crucial, given the OPCW is increasingly conducting missions of a non-routine nature, often with a forensic component.

1

2

3

4

ensics

Objectives

Ascertain the current state of the art of chemical forensics, with particular focus on determining a sample's life cycle, and applying chemical forensics techniques to materials such as storage containers and non-traditional chemical warfare agents

Assess the impact that machine learning and large dataset usage might have on the field of chemical forensics, and predict changes the field may undergo in the next decade

Review methods and procedures relating to sampling and analysis with additional consideration of reproducibility, standardisation, best practices, and information sharing

Determine how the OPCW and its designated laboratories can use this knowledge to augment and improve their capabilities in the field of chemical forensics

TWG in numbers

17 members

15 States Parties represented

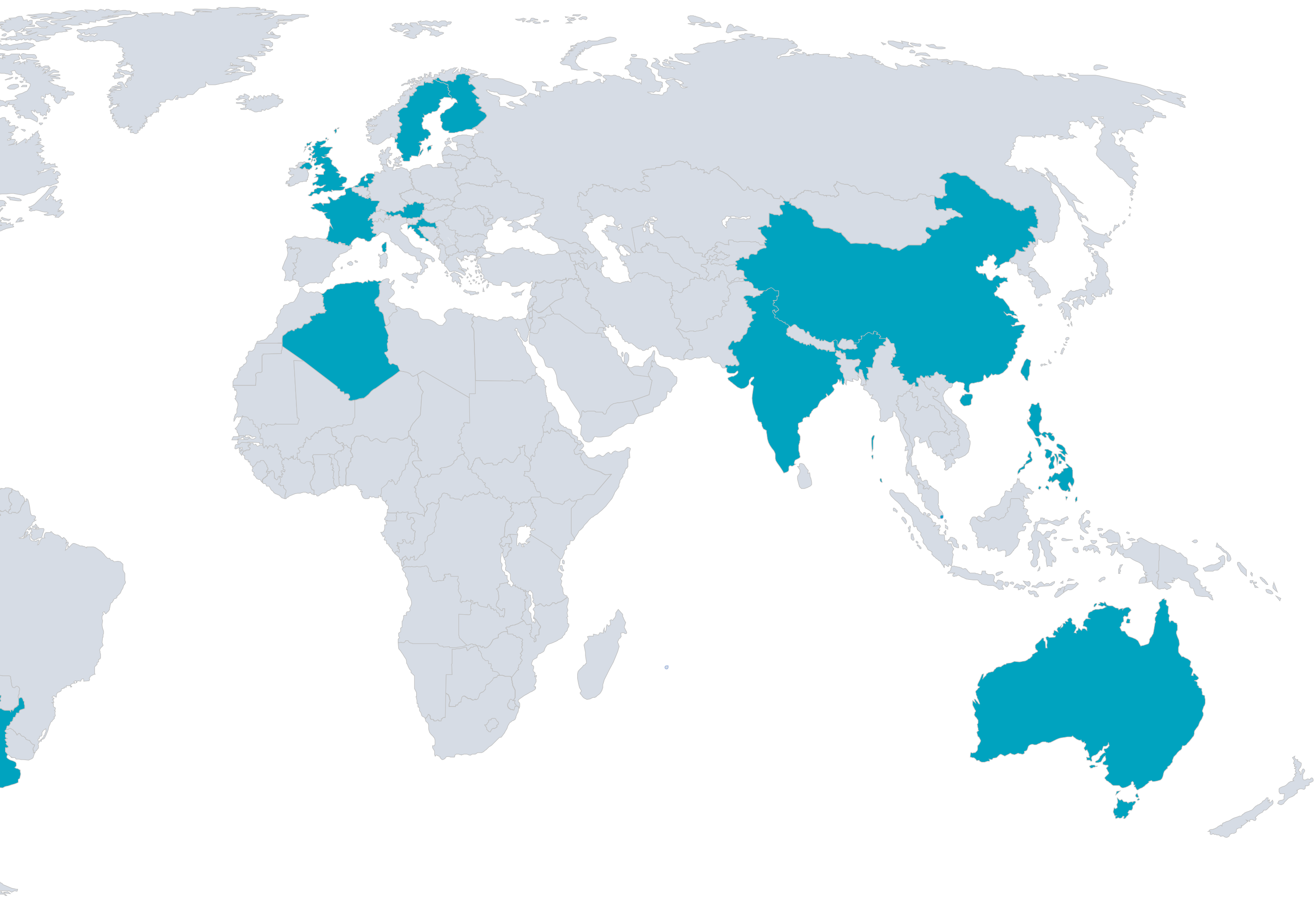
10 external experts

7 current SAB members

9 women

8 men

The boundaries shown in this map do not imply official endorsement or acceptance by the OPCW



Learn more

Scientific Advisory Board's Workshop on Chemical Forensics

Temporary Working Group on Investigative Science and Technology

Temporary Working Group on Analysis of Biotoxins

Follow us

opcw.org

@opcw

@opcw

/opcwonline