Chem-ecting the dots: the world of chemical forensics

Science for Diplomats Series

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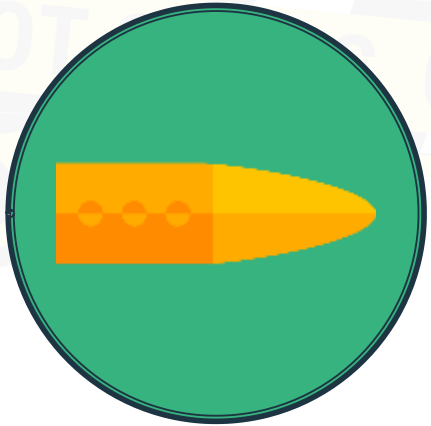
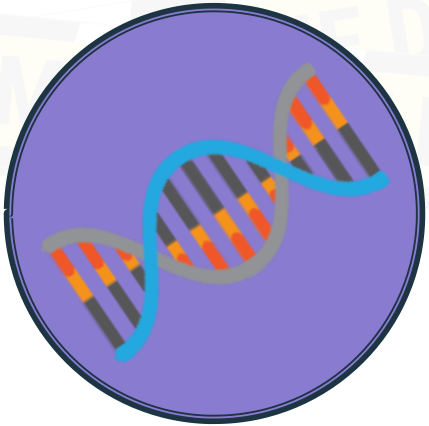
Introduction to chemical forensics

Forensic science

Application of scientific methods and techniques to examine evidence (traces) for investigative purposes



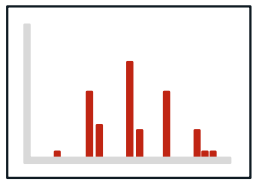


Chemical forensics

Application of analytical chemistry methods and techniques to examine evidence (chemical traces) for investigative purposes

Sample

Distinctive signatures



Impurity profiles

Isotope ratios

Additional information

Production method & location

Impurity profiles

99%

PURITY

Impurities are any chemical species present in a compound that are not the primary or desired component

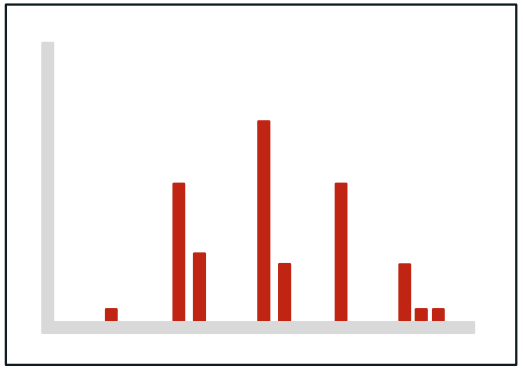
- residual solvents
- catalysts
- unreacted precursors
- byproducts
- manufacturing contaminants
- degradation products

Impurity profiles

99%

PURITY

Impurities are any chemical species present in a compound that are not the primary or desired component



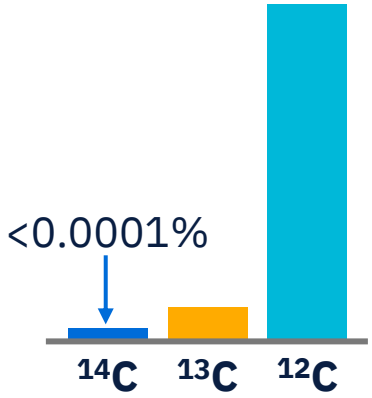
Unique profiles that can be used as forensic signatures

What is an isotope?

Many elements exist in two or more different forms, known as isotopes.

They react in the same way but have subtle differences in their physical properties.

Isotope ratio



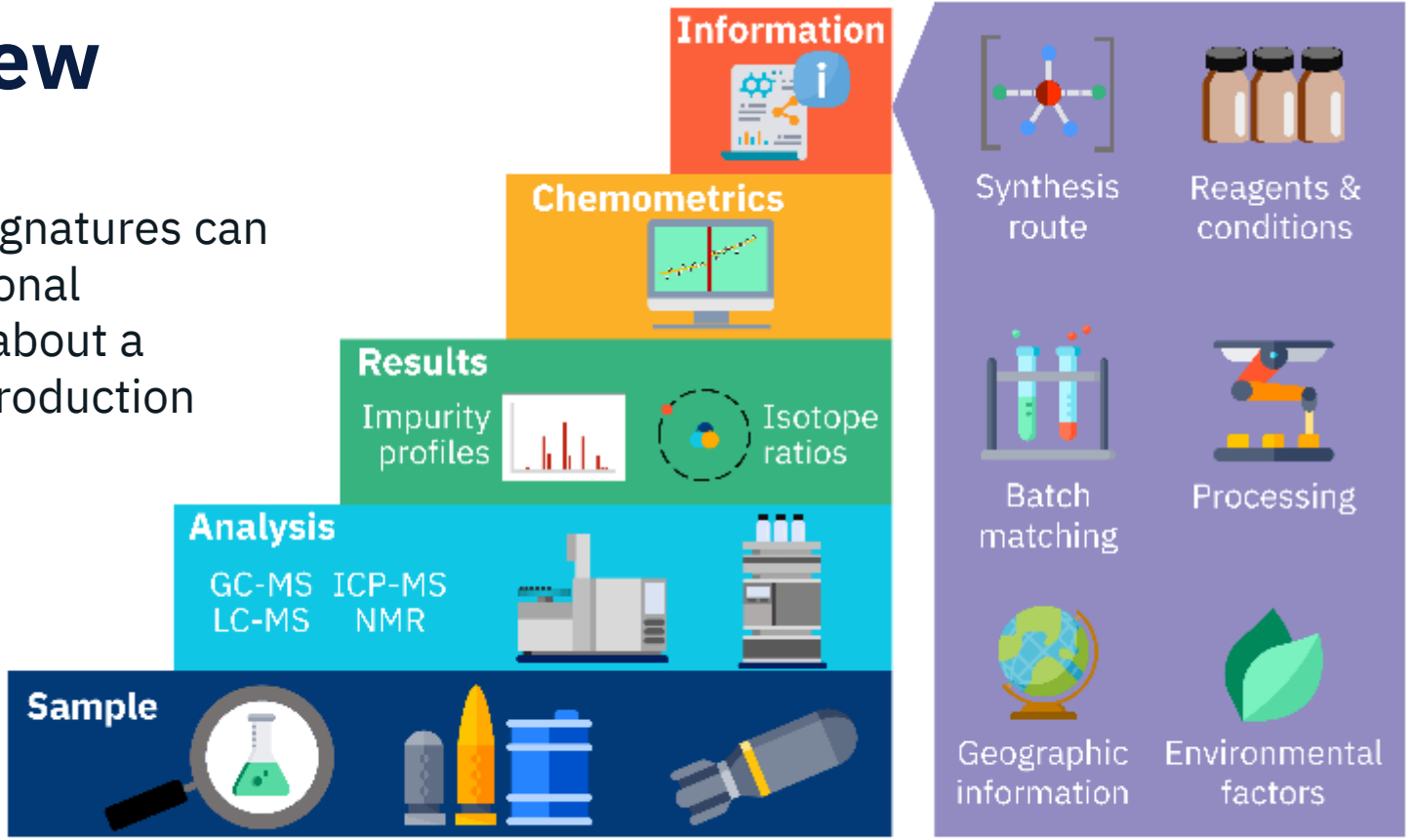
Carbon has 3 isotopes (slightly different forms), present in different amounts.

The different amounts can be measured, giving an **isotope ratio**.

The isotope ratio may be affected by **geographic location and environmental factors**.

Overview

Distinctive signatures can reveal additional information about a chemical's production history



Applications of chemical forensics

Drugs

Illicit drugs

- Signatures related to plant origin enable the provenance of the drugs to be determined
- Impurities provide information about the production method

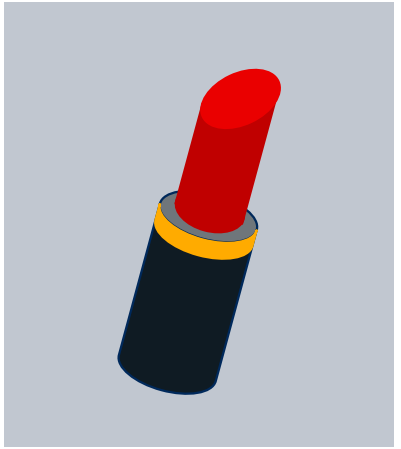
Pharmaceuticals

- Identify counterfeit pharmaceuticals by analysing their chemical composition

Verifying authenticity

Works of art

Food products



Cosmetics

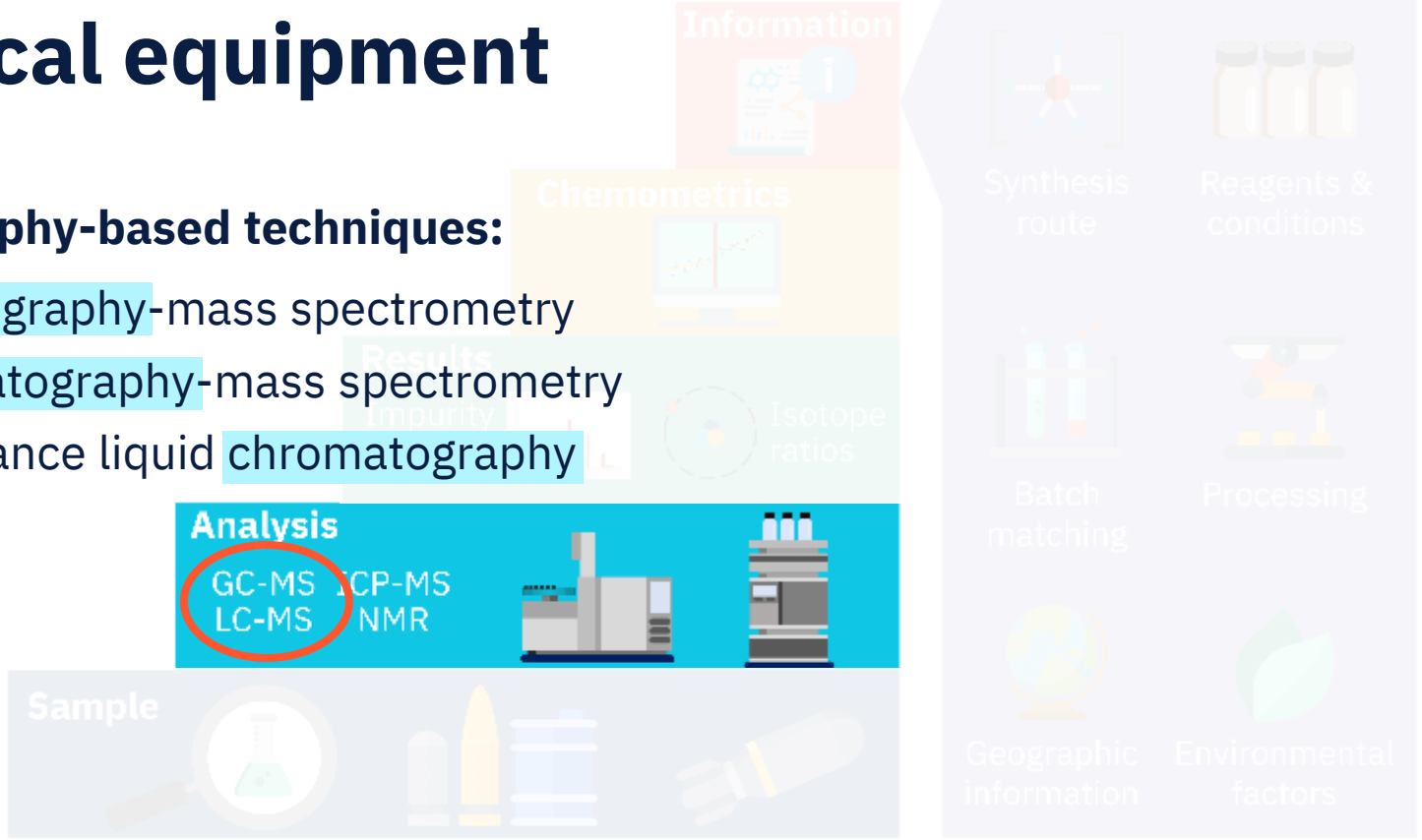
Analytical equipment

Chromatography-based techniques:

Gas chromatography-mass spectrometry

Liquid chromatography-mass spectrometry

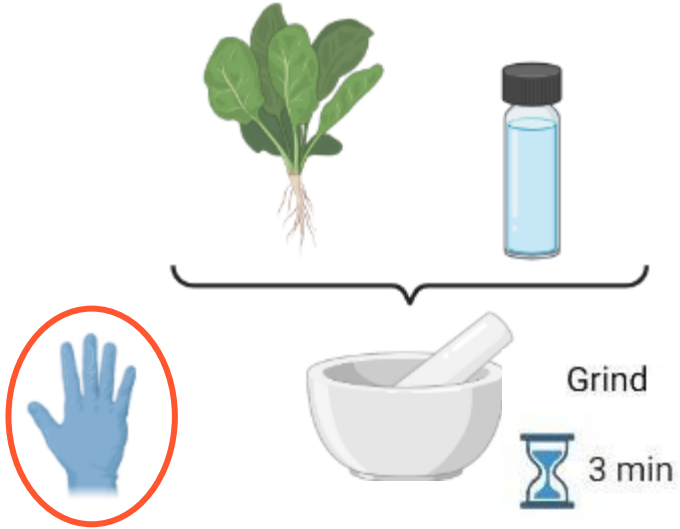
High performance liquid chromatography



Lab time

Thin layer chromatography (TLC)

1



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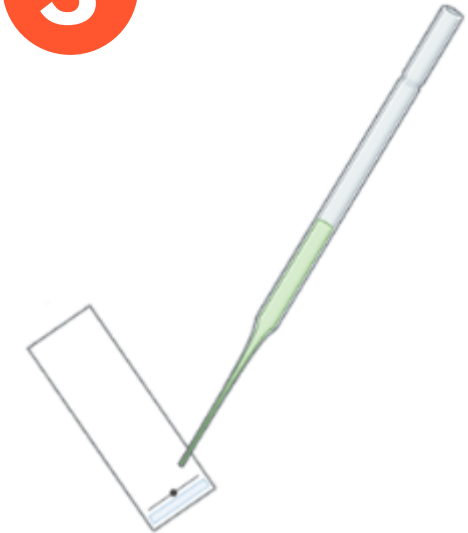


Thin layer chromatography (TLC)

Chromatography 101

Technique which separates mixtures into their individual components

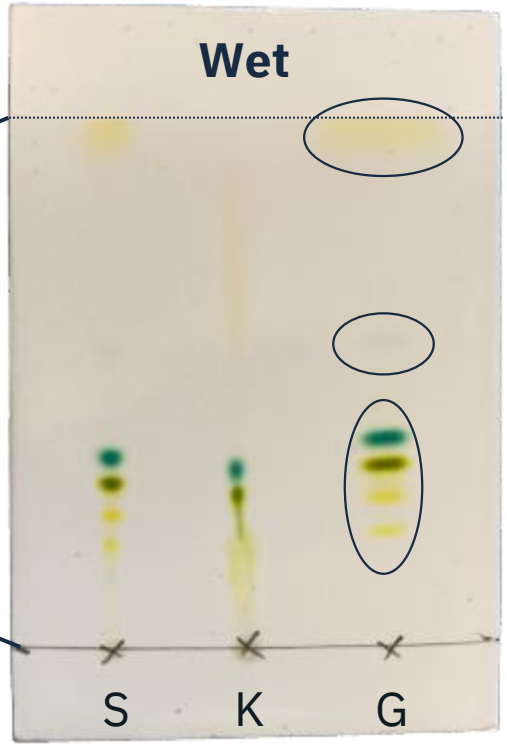
Stationary phase:
a fixed material
Silica gel

Mobile phase:
carries the sample
Acetone and petroleum ether

Components of the mixture are separated according to their affinity for (attraction to) the mobile and stationary phases

TLC results

S = spinach
K = kale
G = grass



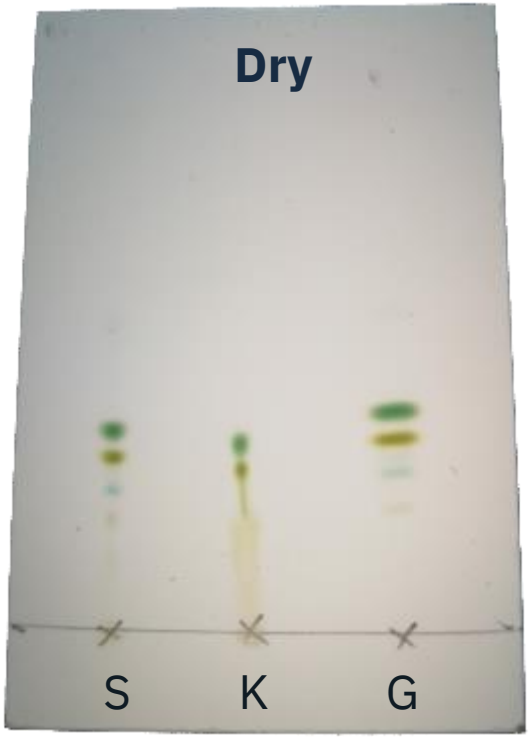
Solvent front

Origin of pigments

Pigment 1

Pigment 2

Pigments 3, 4, 5, 6, (7?)



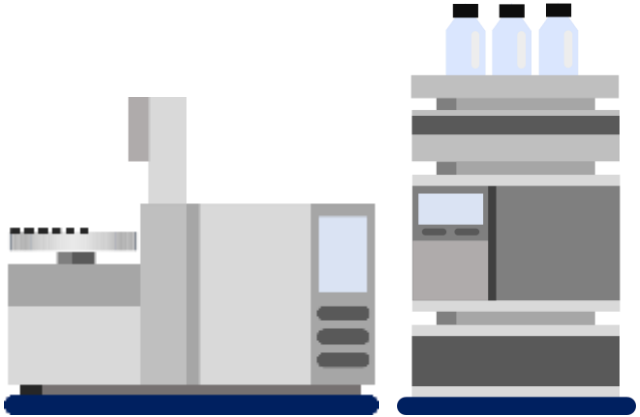
Analytical equipment

Focus on chromatography-based techniques

Analytical equipment

Gas chromatography-mass spectrometry (GC-MS) and **liquid chromatography-mass spectrometry** (LC-MS) are the workhorses of chemical forensics

- “Hyphenated” techniques
- Indispensable for precise and comprehensive analysis
- Selection depends on sample



Analytical equipment

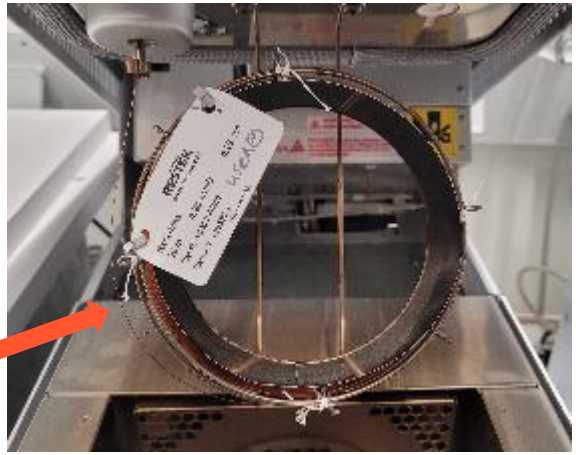
Gas or liquid chromatography	Mass spectrometry
Separates sample mixture into different components	Identifies molecules by “weighing” them
Reduces matrix effects and complexity	Improves accuracy and identification

Demystifying the GC-MS

Autosampler and autoinjector

Sample vials

Demystifying the GC-MS



Column – stationary phase

Mass spectrometer

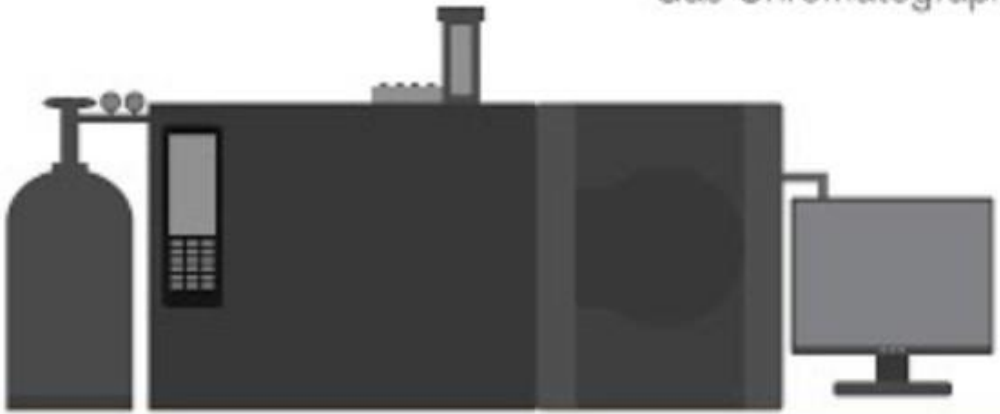
Gas chromatography unit

Transfer line (GC-MS interface)

https://www.youtube.com/watch?v=cBXgSPO3pzw&t=30s

GC-MS

Gas Chromatography Mass Spectrometry

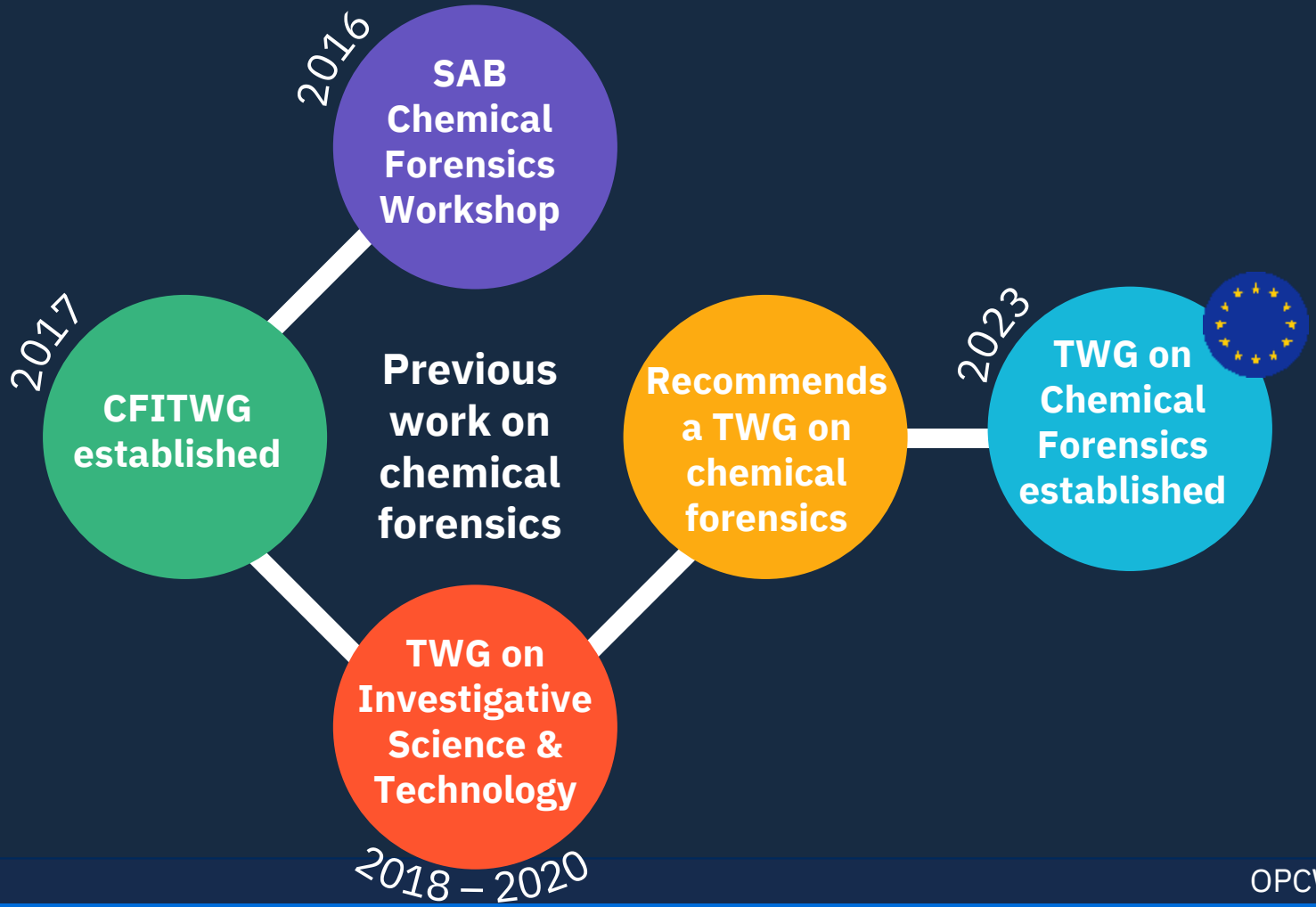


Temporary Working Group on Chemical Forensics

2024 –2026

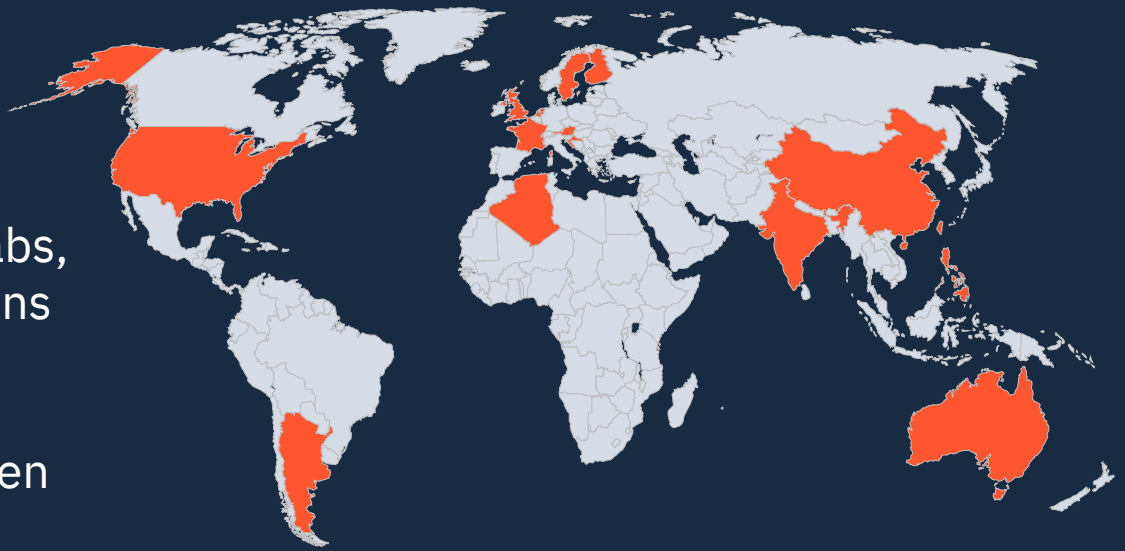
Why have a temporary working group?

The challenge of non-routine missions requires additional capacity and capabilities


2016
SAB Chemical Forensics Workshop
2017
CFITWG established
Previous work on chemical forensics
Recommends a TWG on chemical forensics
2023
TWG on Chemical Forensics established
TWG on Investigative Science & Technology
2018 – 2020

Composition and duration

- 17 members (10 female)
- All 5 Regional Groups represented
- Academia, Designated Labs, International Organisations
- Chair: Anne Bossée
- Vice-Chair: Simon Ovenden



The TWG has a two-year mandate, starting on 1 January 2024

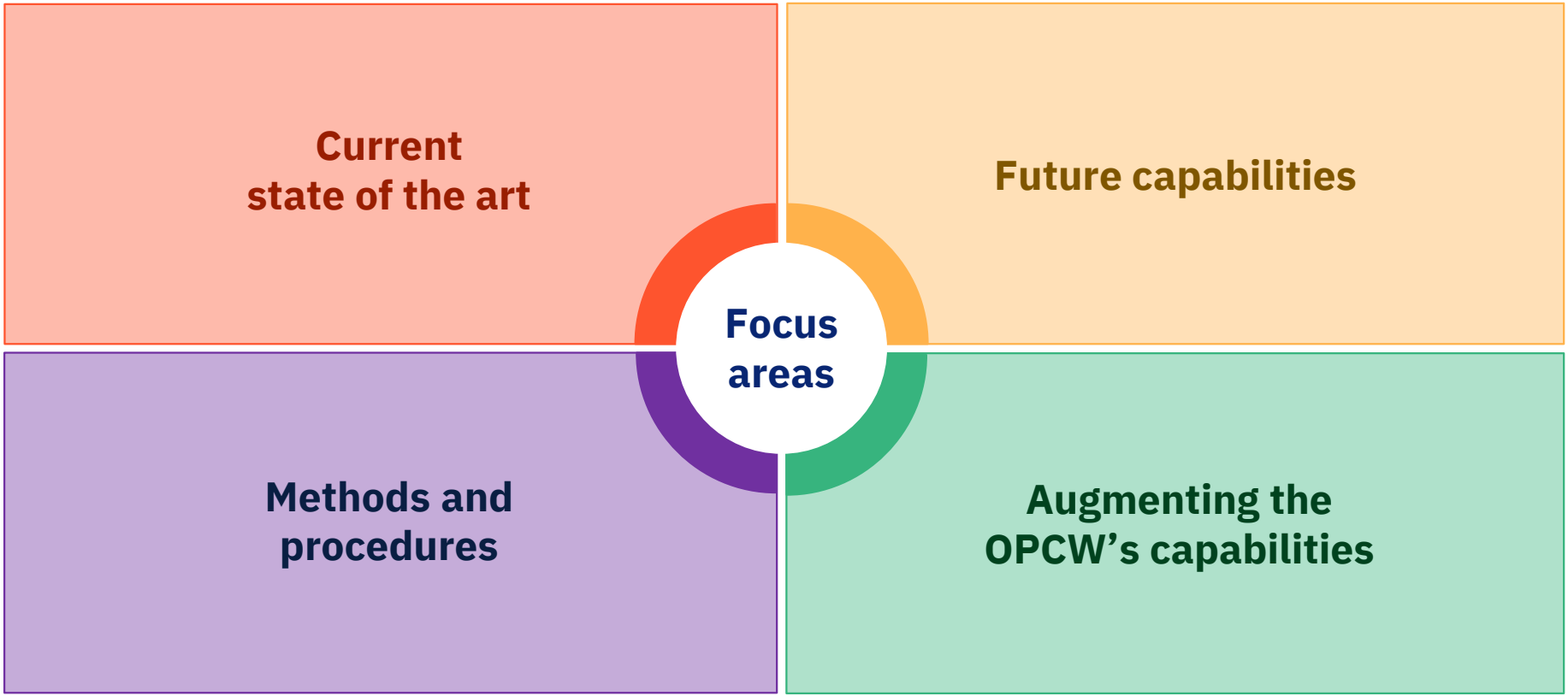
Objectives and operation

Review the science and technology of chemical forensics, identify gaps and limitations

Scan for report

Consider the work and advice of the TWG on Investigative Science and Technology

Provide findings and recommendations to be considered by the SAB and subsequently by the Director-General


Current
state of the art
Future capabilities
Focus
areas
Methods and
procedures
Augmenting the
OPCW's capabilities

Current state of the art

What is the current state of the art related to determining the life cycle of a given chemical sample?

Can analysis of other materials that may be found yield relevant information?

What information is available related to the ability to conduct chemical forensics analysis in other areas and how might this relate to chemical warfare agents?

Future capabilities

How will improved machine learning change chemical forensics?

What impact will limited dataset size have on chemical forensics?

What will the field of chemical forensics look like in 5-10 years?

Methods and procedures

How can applied analytical methods have an impact on the results related to trace analysis and the chemical footprint?

How can data, methods, and procedures be standardised and shared?

What information is needed to ensure trust and reproducibility in the analysis and the results?

How can analytical data from different techniques be combined?

Would curated/shared database(s) be useful? How would they be secured?

What best practices exist for on-site sampling and what challenges remain?

Augmenting the OPCW's capabilities

How can the OPCW…

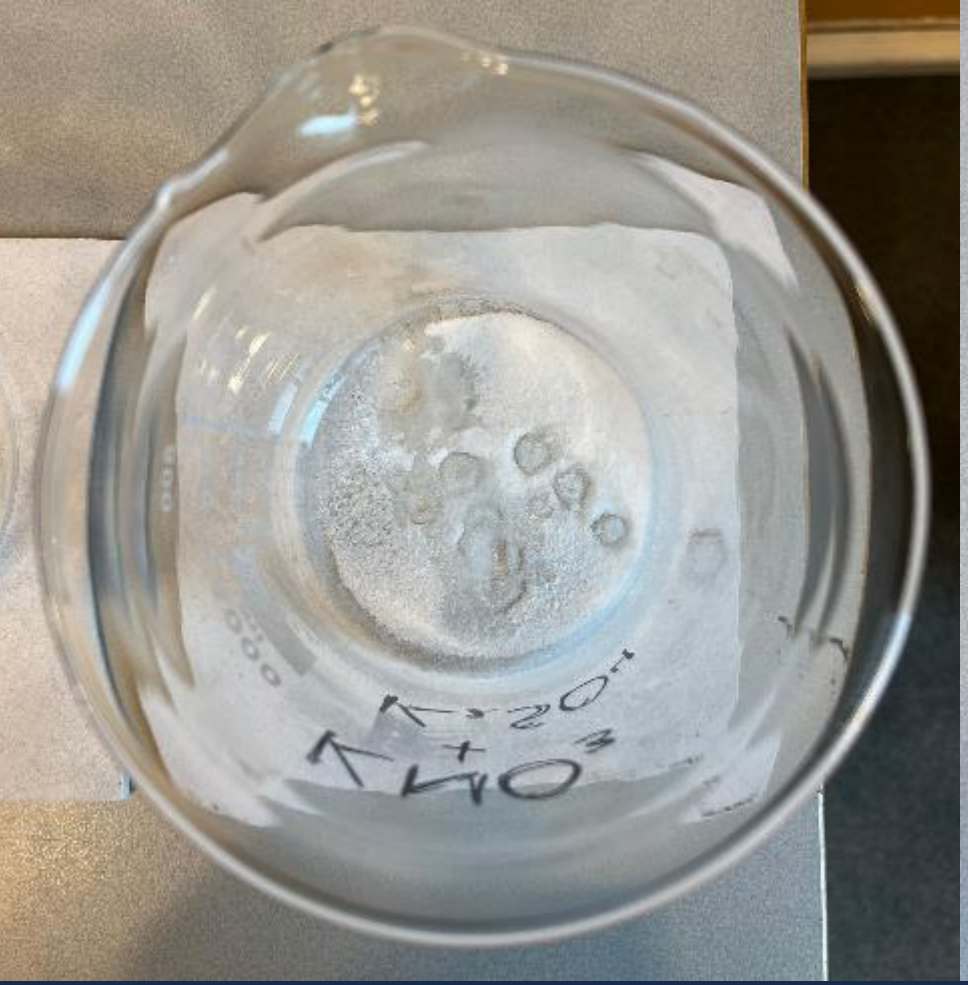
- Improve capture and utilisation of relevant information?
- Ensure and verify the validity of forensic results?
- Ensure that results can be appropriately reported?
- Work with other organisations to augment its capabilities?
- Promote and enhance forensics analysis at designated laboratories?

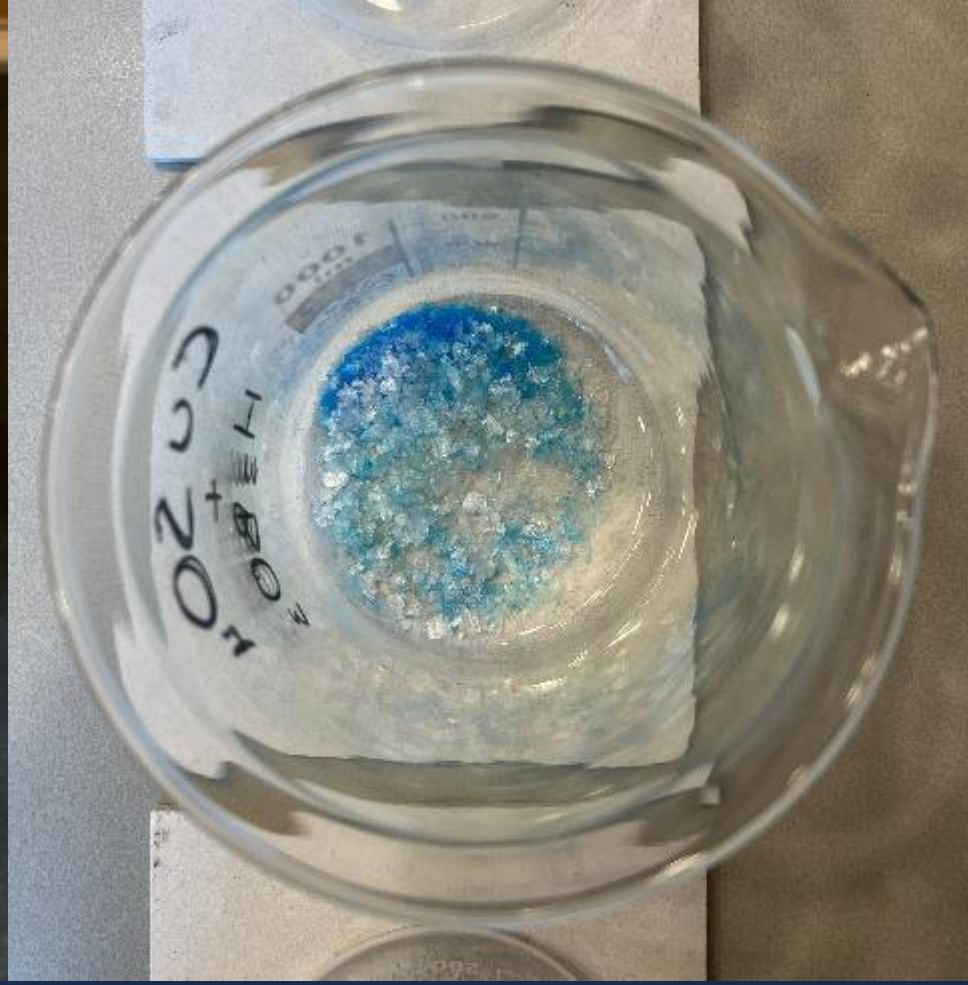





Rainbow flames
demonstration


MgSO4
LiCl
CaCl
1000 ml
NaHCO3
CuSO4
+
H3BO3
1000 ml
KNO3
+
K2SO4
1000 ml


KMnO4


CuSO4

Atomic emission

Metal salts produce characteristic flame colours

- Fireworks
- Sodium streetlights
- Campfires

This property can be used to determine the **elemental composition** of a sample

Elemental analysis

- Determines unique elemental signatures, including isotope ratios
- Complements other chemical forensics techniques
- Corroborates findings to strengthen forensic investigations
- New inductively coupled plasma-mass spectrometry (ICP-MS) instrument at the ChemTech Centre

Elemental analysis

Inductively coupled plasma-mass spectrometry (ICP-MS) instrument

High-performance autosampler

Key takeaways

01

Chemical forensics is the **application of analytical chemistry methods and techniques to examine evidence** (chemical traces) for investigative purposes

02

A range of analytical instrumentation is used to determine distinctive **chemical signatures which can provide important additional information** about a sample

03

The new **TWG on Chemical Forensics will be pivotal for developing a full understanding of the field** and ensuring the OPCW can augment its capabilities in this area

Questions?