Chem-ecting the dots: the world of chemical forensics
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

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

I illicit drugs

Ψ Signatures related to plant origin enable the provenance of the drugs to be determined

Ψ Impurities provide information about the production method

Pharmaceuticals

Ψ 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

Analysis
- GC-MS
- ICP-MS
- LC-MS
- NMR
Lab time
Thin layer chromatography (TLC)

1. Grind
   - 3 min

2. 

3. 

OPCW OFFICIAL
Thin layer chromatography (TLC)

1. Place sample on TLC plate.
2. Develop plate with solvent.
3. Dry plate.
4. Visualize bands under UV light.
5. Monitor for 10 minutes.
6. Record results.

10 min
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

Solvent front

Origin of pigments

Wet

Pigment 1

Pigment 2

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

S = spinach  
K = kale  
G = grass
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

<table>
<thead>
<tr>
<th>Gas or liquid chromatography</th>
<th>Mass spectrometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Separates sample mixture into different components</td>
<td>Identifies molecules by “weighing” them</td>
</tr>
<tr>
<td>Reduces matrix effects and complexity</td>
<td>Improves accuracy and identification</td>
</tr>
</tbody>
</table>
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
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.
Previous work on chemical forensics

CFITWG established

TWG on Investigative Science & Technology

2016

SAB Chemical Forensics Workshop

2017

CFITWG established

Previous work on chemical forensics

Recommends a TWG on chemical forensics

2018 – 2020

TWG on Investigative Science & Technology

2023

TWG on Chemical Forensics established
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

- 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

Methods and procedures

Future capabilities

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

<table>
<thead>
<tr>
<th>Question</th>
<th>Answer</th>
</tr>
</thead>
<tbody>
<tr>
<td>How can applied analytical methods have an impact on the results related to trace analysis and the chemical footprint?</td>
<td>How can data, methods, and procedures be standardised and shared?</td>
</tr>
<tr>
<td>How can analytical data from different techniques be combined?</td>
<td>Would curated/shared database(s) be useful? How would they be secured?</td>
</tr>
<tr>
<td>What information is needed to ensure trust and reproducibility in the analysis and the results?</td>
<td>What best practices exist for on-site sampling and what challenges remain?</td>
</tr>
</tbody>
</table>
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
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
Chemical forensics is the application of analytical chemistry methods and techniques to examine evidence (chemical traces) for investigative purposes.

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

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?

Magnesium  Lithium  Calcium  Sodium  Copper  Potassium