United States Government Accountability Office

Report to Congressional Addressees

September 2023

TECHNOLOGY ASSESSMENT

Chemical Weapons

Status of Forensic Technologies and Challenges to Source Attribution

GAO-23-105439

The cover image displays a potential chemical incident, with investigators collecting samples for forensic analysis.

Cover sources: GAO; Igor/stock.adobe.com (buildings). | GAO-23-105439

GAO

Highlights of GAO-23-105439, a report to congressional addressees

September 2023

Why GAO did this study

Despite the Chemical Weapons Convention's ban on their use, chemical weapons have been used in the past decade in assassinations and on civilian populations. To identify the use of a chemical weapon and then attribute that weapon back to its source, researchers rely on several technologies for chemical analysis. Chemical analysis is one piece of an overall chemical weapon investigation.

This report discusses (1) the status of key technologies available to identify a chemical agent or its source, including their strengths and limitations; (2) challenges researchers and investigators face in trying to identify a chemical agent or its source; and (3) policy options that may help address the challenges of using key technologies to identify a chemical agent and its source.

To conduct this technology assessment, GAO reviewed key reports and scientific literature; interviewed government, intergovernmental, and academic representatives; conducted site visits; and convened two meetings of experts with the assistance of the National Academies of Sciences, Engineering, and Medicine. GAO is identifying policy options in this report.

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TECHNOLOGY ASSESSMENT

Chemical Weapons

Status of Forensic Technologies and Challenges to Source Attribution

What GAO found

When a chemical weapon is used, investigators may use forensic technologies to *detect* that it was used, *identify* the chemical, and help *attribute* it to a likely source. Most technologies for chemical identification are mature. Some technologies for attributing chemical agents based on chemical analyses are under development. For example, a wide variety of laboratory-based and fieldable instruments for chemical identification are in commercial use. Investigators also use data from these instruments to help attribute chemicals to their potential sources, but there are limits to the information existing technologies can provide.

Key technologies to identify and attribute chemical weapons to a likely source

Technology	Information it provides
Chromatography (Gas or Liquid)	Separates and identifies chemicals in a sample mixture. Mature for identification of chemical agents, can inform attribution.
Nuclear Magnetic Resonance Spectroscopy	Determines arrangement of atoms in a molecule. Mature for identification of chemical agents, developing for complex mixtures. Can inform attribution.
Mass Spectrometry	Measures mass-to-charge ratios to identify chemicals in a mixture. Mature for identification of chemical agents, can inform attribution.
Impurity Profiling	Identifies key impurities to link samples to production process or precursor. In development for attribution.
Isotope Ratio Methods	Measures ratio of stable isotopes in a sample to link to a precursor. In development for attribution.

Source: GAO. | GAO-23-105439

GAO found several challenges that can hinder identification and attribution of chemical agents, including the following:

- **Poor samples**: In some instances, investigators cannot obtain useful chemical information because samples are too small, dilute, or degraded.
- **Limited reference data**: Generally, chemical identification methods rely on comparison to data from known chemicals, called reference data. However, reference data can be limited because they are resource intensive to collect, analyze, and archive. Additionally, reference data may be challenging to use in some instances, such as if they were developed using different experimental methods or stored in an incompatible format.
- **Lack of information sharing**: Controls on information sharing are needed for national security concerns but can hinder collaboration among researchers in developing technologies and improving understanding of chemicals and their sources.
- **Limited coordination**: Entities may not be aware of individual and laboratory expertise that could assist with identifying a chemical agent or its source. Researchers may unknowingly duplicate work, and opportunities to strengthen capabilities may be missed.

GAO identified six high-level policy options in response to these challenges. These policy options are provided to inform policymakers of potential actions to address the challenges identified in this technology assessment. They identify possible actions by policymakers, which include Congress, federal agencies, state and local governments, academic and research institutions, and industry.

Policy options to address challenges that hinder identification and attribution of chemical agents

Policy Option	Opportunities	Considerations
Develop technology to aid with sampling (report p. 35) Policymakers could encourage development of technologies that allow more rapid sample analysis or that slow sample degradation.	• Could reduce likelihood of degradation by shortening time between sampling and analysis. • May reduce cost of analysis by minimizing the number of chemical signatures generated by sample degradation.	• Small market size for certain instrumentation may limit industry interest in developing new technologies. • Testing of new technologies can be challenging due to the toxicity and reactivity of chemical agents.
Study known threats (report p. 36) Policymakers could advance scientific knowledge on known chemical agents and threats.	• Could support a faster response to an event and faster attribution to a source. • Could ensure that the U.S. has the appropriate workforce, capabilities, knowledge, and facilities to respond effectively to chemical incidents.	• In some cases, additional knowledge is unlikely to help identify a chemical (e.g., due to highly degraded samples) or attribute it to its source (e.g., when there are many possible production processes for a given chemical agent). • Building the necessary body of knowledge could be resource intensive.
Further anticipate emerging threats (report p. 37) Federal policymakers could foster development of technologies and approaches that help anticipate emerging chemical threats.	• Could deter use of chemical agents and support a faster response in the event of use. • Emerging chemical threat assessment and characterization technologies could better prepare U.S. government entities and international partners for the unexpected.	• A vast number of chemicals are potential emerging threats, and efforts would require careful prioritization. • Computational approaches would require security considerations to protect potentially classified chemicals.
Standardize data (report p. 37) Policymakers could encourage standardization of future data collection and support efforts to modernize legacy data on chemical threats.	• Could ensure that computational methods work on data from different sources, maximizing efficiency and potential insights. • Modernized legacy data may provide insights that are otherwise expensive or difficult to acquire.	• Consensus on standard operating procedures may be difficult to achieve. • Legacy data may be challenging to use in certain circumstances, such as due to changes in experimental design, instrumentation, and analytical techniques over time.
Share information (report p. 38) Federal and international policymakers could facilitate information sharing to increase collaboration on chemical agent forensic analyses.	• Quickly making classification decisions about new and emerging information could improve appropriate research collaboration and information exchange. • Increased understanding of classification guidance could improve handling of classified information and allow researchers to more confidently know what information can be shared.	• Classification systems are complex, and creating tools to assist in navigating them could be challenging. • Agencies need to balance facilitating additional information sharing with protecting information critical to national security.
Coordinate on chemical attribution (report p. 40) Federal and international policymakers could encourage increased coordination between entities involved in chemical attribution.	• Clear roles and responsibilities could enable each entity to quickly execute its mission in response to a chemical incident. • Collective development of robust methods and capabilities could increase international confidence in findings.	• Federal agencies often have different goals and requirements, so efficiencies may be limited, even with increased coordination. • Coordination activities with multi agency participation could divert resources away from other tasks.

Source: GAO. | GAO-23-105439

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Abbreviations

DF	methylphosphonyl difluoride
FFM	fact finding mission
GC	gas chromatography
HRMS	high-resolution mass spectrometry
IIT	Investigation and Identification Team
IR	infrared
JIM	Joint Investigative Mechanism
LC	liquid chromatography
MS	mass spectrometry
NMR	nuclear magnetic resonance
OPCW	Organisation for the Prohibition of Chemical Weapons
PF6	phosphorus hexafluoride
UK	United Kingdom

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Congressional addressees

Chemical weapons have been used in warfare and assassinations in various forms for centuries.[1] According to the United Nations, chemical weapons have caused over a million deaths since World War I. This century, over 1,500 people have been killed by chemical weapons, according to estimates from non-governmental organizations. These weapons can be attractive for use by terrorists, governments, and others because of their debilitating and deadly effects, rapid action, psychological impact, and difficulty to detect, among other reasons. The chemical agents used in chemical weapons can be so toxic that they can have severe health effects before the individual notices they have been exposed. They can also pose long-term hazards—there are still unrecovered chemical weapons in World War I battlefields. The effects of these weapons have led to a ban on their use under the Chemical Weapons Convention.

Despite this ban, chemical weapons have been used since 2013 in Syria, Malaysia, the United Kingdom, and Russia, and the State Department has raised concerns about countries' compliance. In its 2022 report on compliance with the Chemical Weapons Convention, the State Department certified that multiple countries were in non-compliance with the convention (i.e, Burma, Iran, Russia, Syria) and that the U.S. could not certify that China had met its treaty obligations.[2] For example, it stated that Russia retains an undeclared chemical weapons program. The report raised multiple concerns about Russia's program, including concerns that Russia's pharmaceutical-based agent program is for offensive purposes.[3] In the case of China, the report stated that the U.S. has concerns regarding China's research of pharmaceutical-based agents and toxins with potential dual-use applications.[4]

[1]The Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons and on their Destruction (Chemical Weapons Convention) defines chemical weapons as the following, together or separately: a) toxic chemicals and their precursors, except where intended for purposes not prohibited under this Convention, as long as the types and quantities are consistent with such purposes; b) munitions and devices, specifically designed to cause death or other harm through the toxic properties of those toxic chemicals specified in subparagraph (a), which would be released as a result of the employment of such munitions and devices; or c) any equipment specifically designed for use directly in connection with the employment of munitions and devices specified in subparagraph (b). The Convention on the Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons and on their Destruction, Article II, April 24, 1997, available at www.cwc.gov/cwc_treaty.html.

[2]U.S. Department of State, *Compliance with the Convention on the Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons and on Their Destruction Condition (10)(C) Report*, (April 2022).

[3]According to the Department of Homeland Security, pharmaceutical-based agents are a category of chemical threat agents that includes synthetic opioids.

[4]The Organisation for the Prohibition of Chemical Weapons (OPCW), the international organization established by Chemical Weapons Convention to support its implementation, defines dual-use chemicals as chemicals that can be used for peaceful civilian and commercial purposes, but can also be used in the creation of weapons or as weapons.

When a chemical weapon is used, entities, such as the Federal Bureau of Investigation (FBI) or the Organisation for the Prohibition of Chemical Weapons (OPCW), may conduct an investigation. Part of that investigation may involve forensic technologies that can *detect* that a chemical was used, *identify* the chemical, and inform the *attribution* of its use to responsible parties. Attribution refers to identifying the likely source of a chemical weapon (such as stockpiles of a specific government, a terrorist organization's supplies, or homemade material) as well as identification of who used the weapon and how they delivered it. The ability to attribute a chemical weapon to its source helps serve two purposes: (1) holding those who use chemical weapons accountable and (2) deterring potential users by increasing the likelihood that they would be identified.

For purposes of this report, we will focus on technologies for identification of the chemical weapon and to aid in attribution to a likely source. We will refer to a chemical previously used as a weapon as a chemical *agent*, and a chemical with potential to be used for harm as a chemical *threat*. In addition to known chemical threats, there also are emerging threats. We define *emerging threats* as either (1) a new physical form of a known chemical agent, or (2) a brand new chemical threat.

We conducted this work under the authority of the Comptroller General to assist Congress with its responsibilities, in light of congressional interest in attribution of chemical weapons. We examined (1) status of key technologies available to identify a chemical agent or its source, including their strengths and limitations; (2) challenges researchers and investigators face in trying to identify a chemical agent or its source; and (3) policy options that could help address those challenges.

To address all objectives, we reviewed scientific literature, policy literature, agency guidance, and other documents; interviewed agency officials, academic researchers, and laboratory staff, including end users of the technologies; visited the Army Combat Capabilities Development Command Chemical Biological Center, the National Nuclear Security Administration's Lawrence Livermore National Laboratory, and the Department of Energy's Pacific Northwest National Laboratory; and convened two meetings of experts representing a range of perspectives. See appendix I for more details on our scope and methodology and appendix II for a list of participants in our expert meeting.

We conducted our work from September 2021 to September 2023 in accordance with all sections of GAO's Quality Assurance Framework that are relevant to technology assessments. The framework requires that we plan and perform the engagement to obtain sufficient and appropriate evidence to meet our stated objectives and to discuss any limitations to our work. We believe that the information and data obtained, and the analysis conducted, provide a reasonable basis for any findings and conclusions in this product.

1 Background

1.1 Chemical weapon programs

During and after World War I, several countries developed and stockpiled a variety of chemical weapons. The stockpiles reached their peak during the Cold War. In 1997, the Chemical Weapons Convention—a multilateral treaty to which there are currently 192 States Parties, including the U.S.—entered into force.[5] States Parties to the treaty agree that they will not develop, produce, retain, acquire, stockpile, transfer, or use chemical weapons; will destroy stockpiles of chemical weapons and chemical weapon production facilities; and will subject certain chemicals and facilities to declaration, inspection, and verification requirements as specified in the Verification Annex, among other things.[6] Despite this treaty, chemical weapons have been used since 2012 on a scale not seen in decades.

Chemical weapon programs are highly secretive, and access to information about them and the associated chemical agents is controlled. Information related to chemical defense often receives a national security classification for a variety of reasons. Details about specific production routes may be deemed classified or otherwise sensitive, because they could contribute to proliferation of chemical agent production, or help an adversary make a chemical agent that is difficult to distinguish from the same agent made by another entity. This ability could provide plausible deniability or result in false claims following a chemical incident.

The ability to publicly attribute chemical weapons to their source requires, among other things, insight into other countries' chemical weapon programs or similar information. In some instances that information may be difficult to obtain.

1.2 Chemical incidents and investigations

We define a *chemical incident* as the unauthorized use of chemical agents. These incidents could occur in a variety of settings, such as widespread use in international or civil conflicts, use by terrorist organizations, or use in assassination attempts. In the past decade, chemical agents have been used in the Syrian Civil War, in an assassination in Malaysia, and assassination attempts in the United Kingdom and Russia. For selected detailed incident summaries, see section 2.2.

[5]According to the State Department's 2022 report, the U.S. objected to the accession of the "State of Palestine" to the Chemical Weapons Convention and does not consider itself to be in a treaty relationship with the "State of Palestine" under the Chemical Weapons Convention. Therefore, this number does not include the Palestinians.

[6]The Chemical Weapons Convention requires states parties to adopt the necessary measures to implement its obligations under the Chemical Weapons Convention, which includes prohibiting those under its jurisdictions from undertaking any activity prohibited to a state party under the Convention and enacting penal legislation with respect to such activity. In 1998, the U.S. enacted the Chemical Weapons Implementation Act of 1998, as part of the Omnibus Consolidated and Emergency Supplemental Appropriations Act, 1999, Pub. L. No. 105-277, div. 1 112 Stat. 2681, 2856-86. According to the State Department's 2022 report, 74 state parties had not yet notified the appropriate officials of the adoption of implementing legislation and/or regulations covering all of the measures.

Chemical agents can take many forms. Many different chemicals could be used to cause intentional death or harm through their toxic properties, including chemical warfare agents, toxic industrial chemicals, and pharmaceuticals.[7] Chemical agents may be stored as a pure substance or may be made from relatively inert starting materials prior to deployment. Sarin (a clear liquid) is a well-known warfare agent, and chlorine (a yellow-green gas that is denser than air) is a well-known toxic industrial chemical. Pharmaceutical-based agents are chemicals based on pharmaceutical compounds, which may or may not have legitimate medical uses, and can cause severe illness or death when misused. Chemical agents can be solids, liquids, or gases and can be weaponized through many methods. See table 1 for more information about selected chemical agents.

After a chemical incident, many organizations can be involved with identifying and attributing chemical agents to their source as part of an investigation.[8] These organizations include *sponsoring entities*, which may be governments, specific agencies, or an international organization.[9] Some of these entities employ teams to collect samples from an incident site and other sites of interest. Samples can include soil, vegetation, paper, human or animal tissue, or cloth wipes and cotton swabs used to remove whatever material is on a surface of interest (see fig. 1 for selected representative examples).

Table 1: Selected chemical agents

Agent	Chemical Type	Physical Properties	Health Effects	Notable Uses
Sarin	Warfare agent	Clear, colorless liquid	Loss of consciousness, convulsions, paralysis, death	Tokyo Subway attacks (1995), Syrian Government (2012-2019)
Chlorine	Toxic industrial chemical	Yellow-green gas	Nose, throat, and eye irritation, vomiting, lung damage, death	World War I, Syrian Government (2012-2019)
Fentanyl derivatives	Pharmaceutical-based agents	Varied, generally white solids	Respiratory arrest, disorientation, sedation, death	Dubrovka theater hostage crisis (2002)

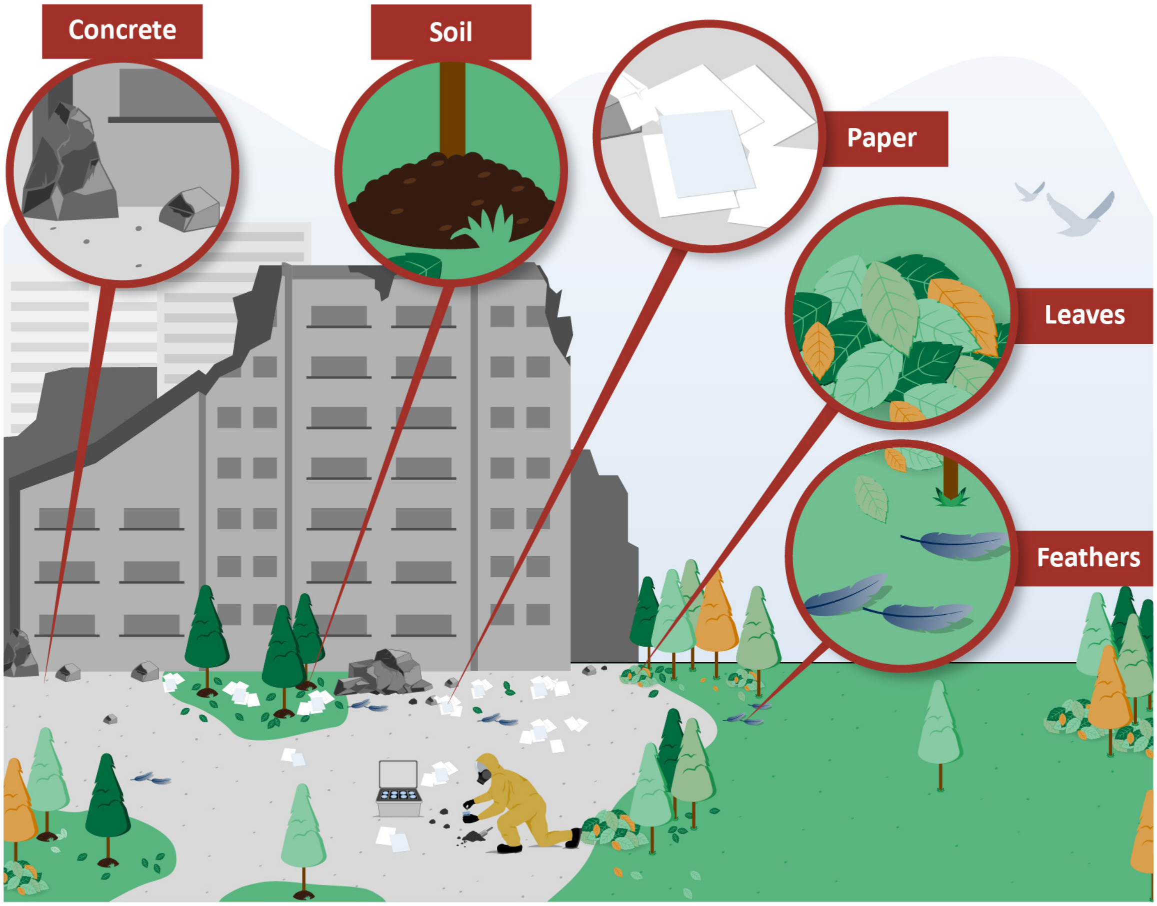
Source: GAO analysis of government agency information. | GAO-23-105439

[7]Chemical warfare agents are chemical agents developed for military use.

[8]Forensic chemical investigations may not only occur after a publicly known incident, but we focus on that scenario for simplicity.

[9]Part XI of the Verification Annex to the Chemical Weapons Convention addresses OPCW investigations in cases of alleged uses of chemical weapons initiated pursuant to Articles IX or X of the Convention and discusses matters such as the request for an inspection of an alleged use of chemical weapons in the territory of a state party, the assignment of an inspection team, and the conduct of investigations.

Figure 1: Examples of how investigators collect a variety of samples from incident sites for forensic analysis



Source: GAO. | GAO-23-105439

Sponsoring entities also commission laboratories to analyze samples. These laboratories also develop new methods—and in some cases, new technologies—to identify and attribute chemical agents to a source. Some laboratories are *chemical surety laboratories*, which can handle pure chemical agents and samples containing them. Some surety laboratories are designated by the OPCW to conduct analyses.[10] Other laboratories, including some government and academic laboratories, may work with small amounts or low concentrations of chemical agents or with surrogate materials to develop methods that could be used by surety labs during investigations. Table 2 describes relevant roles of selected organizations.

[10]OPCW-certified laboratories may be commissioned to perform off-site analysis of chemical samples collected by OPCW inspectors from chemical production facilities, storage depots and other installations, or from the site of an alleged use of chemical weapons.

Table 2: Selected organizations involved with identification and attribution of chemical agents

Organization	Key roles relating to chemical agents
Centers for Disease Control and Prevention	Has a laboratory designated by the OPCW for the analysis of authentic biomedical samples. Provides training to U.S. labs to detect biomarkers associated with human exposure to chemical agents.
Department of Defense[a]	Has procedures for responding to a chemical event and laboratories that can analyze chemical agent samples. One Department of Defense laboratory is designated by the OPCW for the analysis of authentic samples.
Department of Energy	Has a laboratory designated by the OPCW for the analysis of authentic biomedical and environmental samples and other laboratories with the capacity to analyze chemical agents in small quantities for research or forensic purposes.
Department of Homeland Security[a]	Detects chemical threats coming into the U.S. and within the respective areas of responsibility of Department of Homeland Security components and prepares for response and recovery.
Department of State	Responsible for promoting, overseeing U.S. implementation of, and assessing compliance with the global ban on chemical weapons. Develops policies to address emerging chemical agent issues and challenges. Federal agency that houses the U.S. National Authority for the Chemical Weapons Convention.
Federal Bureau of Investigation[a]	The lead U.S. federal agency for investigating and collecting intelligence on domestic chemical threats and incidents, and for investigating use of chemical agents against US citizens and interests abroad.
Intelligence agencies[a]	Work to prevent the creation and proliferation of chemical weapons.
Organisation for the Prohibition of Chemical Weapons (OPCW)[a]	International organization overseeing global efforts to eliminate chemical weapons pursuant to the Chemical Weapons Convention. In 2018, the OPCW established the Investigation and Identification Team (IIT) to attribute responsibility for chemical weapons use in Syria. Designates labs through annual proficiency testing and commissions those labs to analyze chemicals for OPCW investigations.

Source: Agency officials and adapted from relevant agency websites. | GAO-23-105439

[a]Denotes entities that sometimes sponsor investigations of chemical incidents.

1.3 Chemical forensic analysis

Chemical forensic analysis involves analyzing the samples collected at an incident site in a laboratory and providing data for use in the wider investigation. Samples often contain numerous chemicals in addition to the chemical agent itself, all of which are important to the analysis. For example, *precursors* are chemicals that are used as starting materials to make a chemical agent. The chemical industry produces thousands of precursors. *Degradation products* are different compounds formed from the agent as it degrades or reacts with other materials or even with itself.

To conduct a forensic chemical analysis, scientists use several technologies to gather data on any chemicals that are present. This process involves four steps:

- **Sample collection:** Described above.
- **Sample preparation:** Treatments to extract chemicals of interest from a sample or render a sample suitable for analysis.
- **Analysis:** Measurement using a variety of instruments to determine the composition and quantity of the chemicals present.
- **Data interpretation:** The interpretation of data from the analysis step, often by comparison with data from known chemicals and processes, referred to as *reference data*.

Scientists use this process to answer questions from a sponsoring entity. The questions chemical analysis may be able to answer include the following.

Is or was a chemical agent used, and what is it? Several technologies can help determine if a chemical agent is or was present in an area. These range from rapid response technologies that inform quick decisions in the field, to highly sensitive technologies used in a lab for trace analysis. Data from these technologies can inform decisions such as what countermeasures to deploy, where to collect samples, and whether to conduct further forensic investigations.

What are the threat characteristics of a chemical? Answers to this question inform decisions about prioritizing threats and developing countermeasures. For example, chemical analysis can help determine whether chemicals present a toxicological risk, how they affect the human body or otherwise cause damage, how long they may persist, whether they are easy or difficult to weaponize, and whether treatment or other countermeasures are available for people exposed to them.

How was a chemical agent made? Analytical techniques can help determine the level of sophistication of preparation of a chemical agent and the *synthetic route*—the process used to produce the agent (see text box). While challenging to determine, answers about how a chemical was made provide context for intelligence gathering and law enforcement decisions.

Key concept: Synthetic route

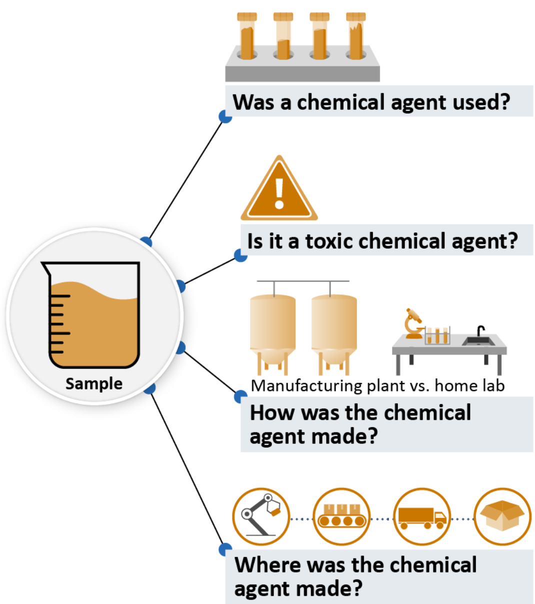
Synthetic route refers to how a chemical agent is made, including the precursors, methods, and equipment used. Information about synthetic routes is important because it can provide clues about the materials used to create a chemical agent, how large the production process was, and an actor's level of sophistication—ranging from an individual with rudimentary knowledge and equipment to a sophisticated nation-state actor with dedicated laboratories and production facilities.

Most chemical agents can be made via a number of synthetic routes. Investigators may research multiple synthetic routes to better understand the chemicals present in samples they examine. For example, a 2021 Swedish Defense Research Agency study on sulfur mustard impurities investigated 11 different synthetic routes. Such studies can help investigators identify or rule out potential sources.

Source: GAO review of literature; Holmgren et. al., "Route Determination of Sulfur Mustard Using Nontargeted Chemical Attribution Signature Screening", Anal. Chem. 2021, 93, 4850−4858. | GAO-22-105439

Where was a chemical agent made? Researchers are developing approaches to determine where a chemical or its precursors were made. For example, chemicals from different regions or suppliers can retain isotopic information throughout the process used to make a chemical agent.[11] Information about the sources of an agent and its precursors may influence diplomatic or legislative actions, as well as strategic planning.

Figure 2: Example questions chemical analysis may be able to answer



Source: GAO. | GAO-23-105439

1.4 Chemical analyses are one part of a forensic investigation

Chemical analyses form one part of a forensic investigation, sometimes along with many other forms of evidence reviewed by multiple organizations. For example, if a chemical weapon projectile were recovered from an incident, investigators could check for DNA, human fingerprints, and labels, in addition to analyzing chemical samples. They would also use metallurgy and other forensic methods to determine the source of the projectile. In a real-world example, the investigation of an attack on the town of Khan Shaykhun during the Syrian Civil War relied on photographs, videos, satellite images, data on wind direction and speed, autopsy results, and crater analysis, in addition to chemical analysis.

Depending on the circumstances, multiple organizations may inform an investigation. In an international context, evidence—including chemical samples—may be provided by a variety of organizations, including the U.S. or other countries' intelligence communities, national militaries, international organizations, non-governmental organizations, and local entities.

Although chemical analyses are just one part of a forensic investigation, they can be used to rule out hypotheses about an incident. Medical reports can provide investigators evidence of the type of chemical agent used in an incident, but chemical analysis is needed to accurately identify specific chemical agents or a chemical agent's likely source.

According to an expert we interviewed, the standards of evidence investigators apply for chemical agent attribution purposes depend on what agency or entity is the lead, the decision-maker's goals, and the context of the chemical incident. These standards dictate how laboratory analyses are conducted. For example, if the agency function and goal is to use the attribution conclusions as part of a prosecution in court, evidence—including chemical analysis—would need to meet the applicable evidentiary standard for

[11] Isotopes are atoms with the same number of protons but different numbers of neutrons.

admissibility of the court. The expert explained that, in contrast, if the results will not be used in court, the evidence and attribution conclusions may be evaluated through the analysts' level of confidence in the conclusions. The conclusions may then inform policymakers' choice of a range of possible actions, such as military action or sanctions. Standards of evidence are inherently more stringent when severe action is being considered.

2 Most Technologies for Identification Are Mature, and Technologies for Attribution Are Emerging

Most technologies for chemical agent identification are mature and provide extensive chemical information from samples, but have limitations. These technologies include a wide variety of laboratory-based and fieldable instruments, many of them commercially available.

Emerging technologies could address some of the limitations, as well as provide data useful in attributing a chemical agent to a known source. Methods for attributing chemical agents based on chemical analyses continue to mature.

2.1 Most technologies for identifying chemical agents are mature but have limitations

Technologies to analyze chemical agent samples are generally mature and commercially available. Table 3 describes some of these key technologies briefly. For more detailed descriptions, see appendix III.

Table 3: Selected technologies for analyzing chemical agents

Technology type	Technology	Abbreviation	Use
Chromatography	Gas chromatography	GC	Separates components in a mixture. Enables identification of chemicals present in samples. Used in combination with mass spectrometry.
	Liquid chromatography	LC	
Spectrometry	Mass spectrometry	MS	Converts chemicals to ions and measures mass-to-charge ratios. Enables identification of chemicals present in samples.
Spectroscopy	Nuclear magnetic resonance	NMR	Determines groupings of atoms in molecules
	Infrared	IR	
	Raman	Raman	

Source: GAO analysis of information from the National Institutes of Health and commercial industry. | GAO-23-105439

Key concept: Mobile analysis: Taking the lab to the incident site

Chemical analysis may be carried out in mobile laboratories, which place scientists closer to an incident site and can cut down on the time between an incident and chemical analysis. Field-deployable laboratory equipment can analyze a sample quickly after an incident, which can preserve chemical information that might otherwise be lost during collection and transport. For example, Army 20th Chemical, Biological, Radiological, Nuclear, Explosives Command officials told us they maintain mobile laboratories with two levels of analytical capabilities to identify chemical agents in the field. Some analytical instrumentation has been miniaturized for portability, though these instruments may not be able to detect trace amounts of an agent as well as laboratory-based instrumentation. Commercially available portable instruments include small Nuclear Magnetic Resonance (NMR) spectrometers and handheld IR and Raman detectors. Some laboratory-based analytical instrumentation can be transported to the field, though field laboratory conditions may not be as controlled as a traditional laboratory, which can reduce instrument sensitivity.

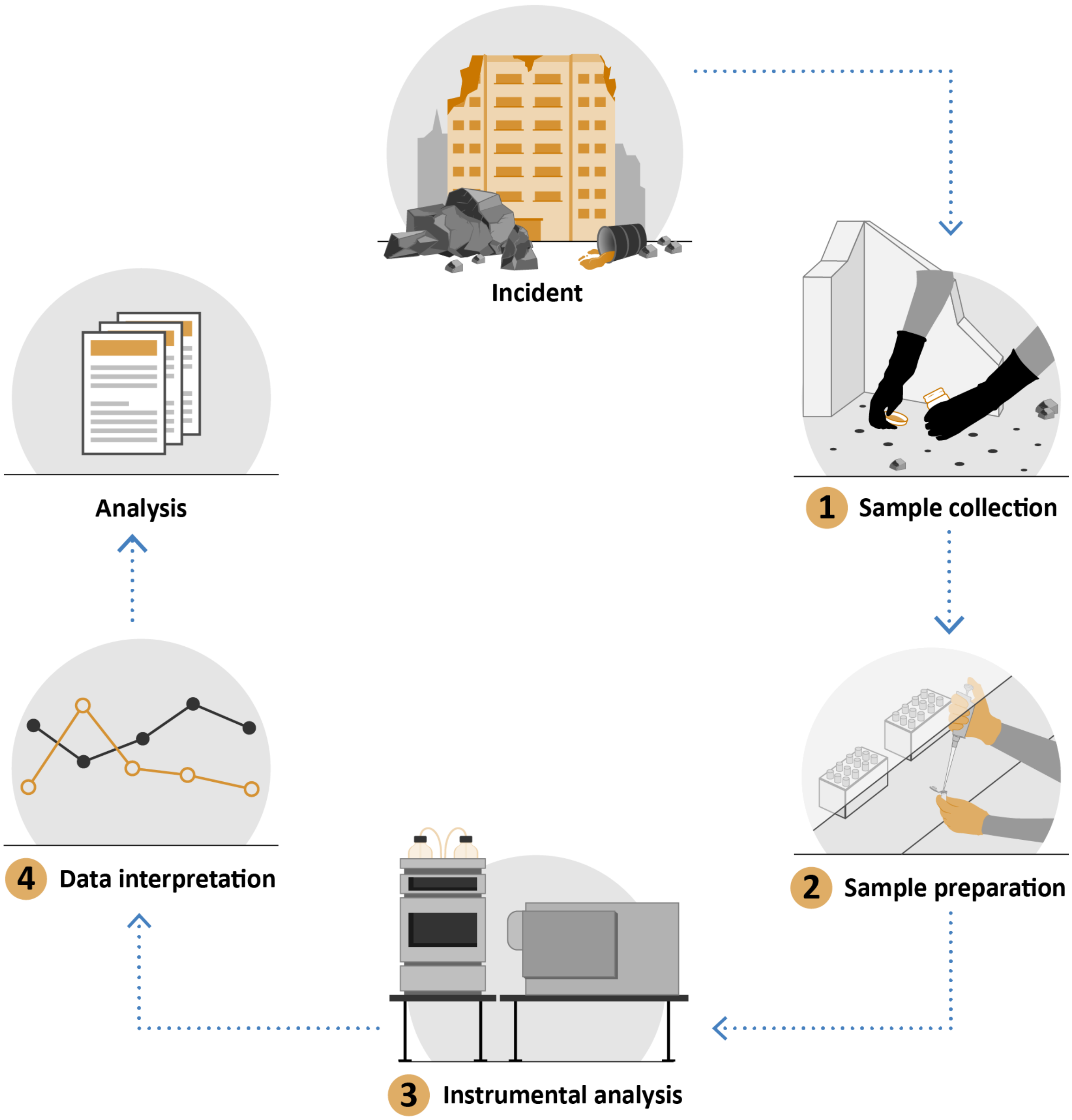
Source: GAO analysis of information from experts. | GAO-22-105439

During an investigation, scientists gather and analyze chemical data from incident samples through a four phase process. In this section, we include an overview of each of these phases, including what they are, how they work, technical challenges, and future prospects. We based this overview on our review of scientific literature, interviews with officials and researchers, and two meetings of experts.

The four phases are:

1. sample collection, in which investigators identify and collect incident samples;
2. sample preparation, a sometimes multi-step process that readies samples for analysis;
3. instrumental analysis, in which scientists examine samples in a laboratory;
4. data interpretation, in which scientists compare processed data to reference data, or create new materials (and phases 2 through 4 applied to these materials) to verify lab results.

Figure 3: Phases in a chemical forensics investigation



Source: GAO adaption of Mene Creative/Kiira Koivunen. | GAO-23-105439

Vignette

SAMPLE COLLECTION

Sample collection methods and technologies vary widely and are informed by situational awareness or other intelligence

What is it?

Multiple experts told us that sample collection is one of the most difficult steps in an investigation, and that ideal collection is often impossible. Samples may be collected at the site of an incident, or another location of interest, with the goal of transporting an informative and well-preserved sample to a laboratory. This operation can be logistically complex. In some cases, before arriving, investigators need information about the conditions and potential hazards at a location, and they may need permission from a government or other entity to access the incident site. They must bring appropriate equipment, plan for sample and other evidence collection, understand where to collect samples that are most likely to contain chemical agent, and arrange for safe and secure transport of samples. An ideal operation 1) immediately collects samples using trained personnel and standardized procedures; 2) thoroughly documents how, when, and where the sample was collected; 3) establishes and documents a secure and complete record of sample handling and management; and 4) transports it with minimal opportunity for contamination and degradation.

Source: GAO (header); Pakhnyushchyy/stock.adobe.com (background image). | GAO-23-105439

How does it work?

The methods used to collect samples depend on the nature and location of an incident, and on the personnel and supplies available. Chemical agents themselves are often a small component of a larger sample mixture, called a matrix. Example matrices include fluids or tissue from human victims, tissue from animals, and soil or vegetation from an incident site.

A variety of technologies can be used to detect and test for the presence of chemical agents at a site, including color-changing paper and handheld detectors. Investigators may also use other technologies, including portable detectors that can take measurements from a distance, called stand-off detectors. Detectors used in the field can be used to inform sample collectors of good sampling locations.

Examples of current and potential future sample collection technology

Source: GAO. | GAO-23-105439

SAMPLE COLLECTION

Key Challenges

- **Choosing a sampling location:** It can be challenging for investigators to know where chemical agents may persist at an incident site, and therefore what locations and materials to sample. Factors like weather can influence where it is best to sample. Chemical investigations can be carried out in a variety of settings, and nearly any material could be sampled as evidence.
- **Samples collected by untrained personnel:** Trained investigators may not be the first to access an incident site, and samples may be collected by untrained personnel. One expert noted it was possible to collect the wrong sample, or to collect the right sample in the wrong way. In either case, the result may be a sample that is insufficient or unsuitable for chemical analysis.
- **Limited utility of handheld detectors:** On-site testing for the presence of chemical agents with handheld detectors can be helpful in informing sampling. But these detectors can only detect what they are programmed to, many are not highly sensitive, and many falsely identify non-threat chemicals as dangerous. As a result, they may not accurately report the presence of some chemicals, such as emerging threats.

Future Prospects

Remotely operated systems: Remotely operated systems for analysis or transport of chemical samples could avoid the need to deploy personnel to an area of concern, reducing risk to personnel and time between an incident and analysis. For example, one Army laboratory has built a sample collection system mounted on a drone. However, these systems may only be able to collect certain kinds of samples.

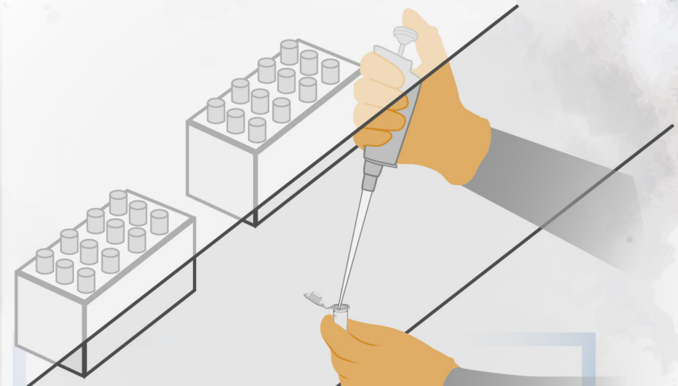
Biomarkers for volatile agents: Highly volatile chemical agents, like chlorine disperse rapidly and do not leave degradation products at an incident site. As a result, many environmental samples from the location may not yield useful information. Researchers are developing methods to identify longer-lasting signs of exposure to volatile chemical agents, known as biomarkers, in vegetation or biomedical samples.

Technologies to determine sampling locations: Technologies developed to inform sample collection could facilitate better identification of sampling location points, potentially enabling collection of samples with higher concentrations of the chemical agent. These could include augmented reality headsets, advanced imaging and detectors, or pre-collection modeling of an incident site. Experts told us sample collection points are informed by an understanding of the surrounding environment. They also stated that further research could improve understanding of where and what to sample as time passes, including types of materials in which chemical agents and associated trace chemicals may persist or be concentrated. Technologies from other fields may be leveraged to accomplish this, including advanced detection systems and environmental modeling. However, some technologies have inherent limitations: for example, it can be difficult to detect low concentrations of chemical agents at a real-world incident scene without prior background scans of the area.

Improved sample containers: Experts told us improvements in sample containers might mitigate sample degradation that may occur.

= Near term   = Longer term

Source: Pakhnyushchyy/stock.adobe.com (background image); GAO (icons). | GAO-23-105439



Vignette

SAMPLE PREPARATION

Sample preparation technologies are well established, but procedures can be time consuming and do not exist for every sample

What is it?

Sample preparation is a set of physical and chemical treatments carried out in a laboratory. Most of the instruments used for chemical forensics require some degree of sample preparation to extract chemicals of interest or prepare samples for analysis. Preparation ensures that the material to be examined is: 1) in a form the instrument can analyze without being damaged, 2) as clean and free of interferences as possible, and 3) representative of the sample. Most individual steps are common practice and have been used for decades, though procedures have not been developed for all chemical agent/matrix combinations.

Scientists consider a variety of factors when developing preparation methods. These factors include the information sought by the sponsoring entity, the limitations inherent in each sample (e.g., the quantity and type of sample), the instruments that are available to scientists, and the kinds of reference data available for comparison.

Source: GAO (header); Pakhnyushchyy/stock.adobe.com (background image). | GAO-23-105439

These methods can be complex, tedious, and time-consuming, in some cases accounting for more than half the laboratory time required to analyze a sample.

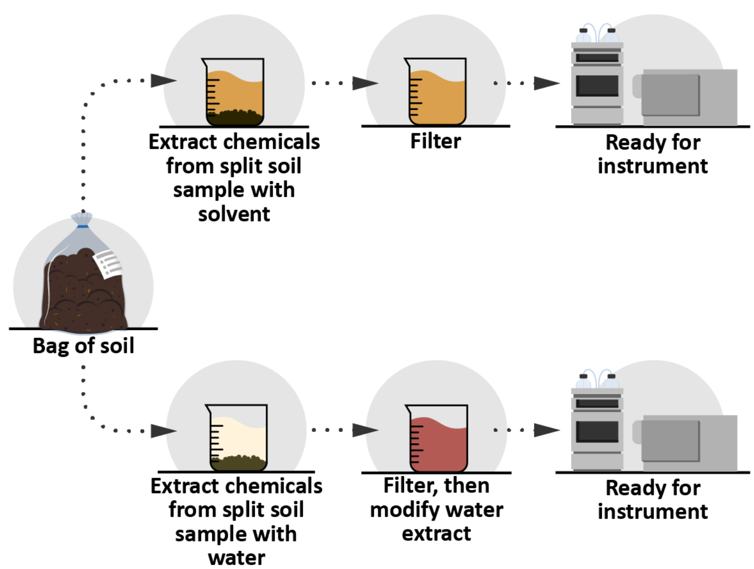
How does it work?

There are many options for sample preparation, such as:

- Homogenization: Blending sample material to ensure that chemicals are evenly distributed throughout.
- Extraction: Washing samples with solvents to separate chemicals by physical properties.
- Modification: Chemically converting sample components to allow analysis with specific instruments.

Sample preparation methods are tailored to the sample the laboratory receives. An example sample preparation procedure for soil, which is one type of material that may be received, is shown below.[12]

Sample preparation requires many steps before the sample can be tested



Source: GAO. | GAO-23-105439

[12] Paula Vanninen, *Recommended Operating Procedures for Analysis in the Verification of Chemical Disarmament*, 2017 edition (University of Helsinki, 2017).

SAMPLE PREPARATION

Key Challenges

- **Sample diversity:** Sample preparation is challenging because samples differ widely in composition and may contain chemicals that interfere with analysis, among other complications. Procedures exist for broad categories of sample types (e.g., solid, liquid, air), but individual samples are likely to present unique challenges. For example there are tens of thousands of different soil types, and each may require a different preparation method. Some of those methods may need to be developed at the time of the sample preparation for analyzing an incident sample.
- **Fidelity:** Each step in a procedure could lead to contamination or loss of chemical compounds of interest, so it is important to use as few steps as possible to prepare a sample while still customizing the steps based on the sample characteristics and target compounds.
- **Reproducibility:** Preparation processes and procedures should be tested multiple times with the same sample during method development to ensure that they produce consistent results before they are applied to incident samples
- **Workforce and facilities**: Incident samples require technical expertise and knowledge, continuous collaboration with instrumentation operators, and timely access to laboratory space and instrumentation.

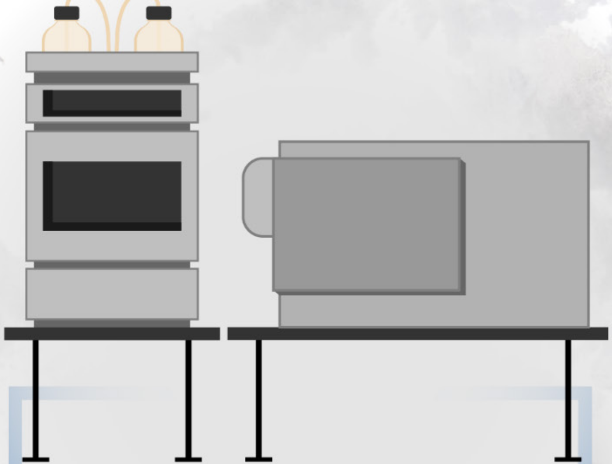
Future Prospects

Automated methods: Robotic systems are in use in some fields, such as pharmaceuticals, and may improve or expedite some sample preparation steps for chemical forensics. Automated methods use robots to perform pre-determined preparation steps for repetitive analyses of known samples, such as repeated analysis of an aging sample. However, robotic sample preparation techniques have not been widely adopted for use in chemical forensics and may not be well-suited because of the wide variety of samples that may come to a laboratory.

Preparation-less techniques: Some analytical methods could benefit from no or minimal preparation to cut down on the amount of time before analysis. Traditional sample preparation techniques use a variety of solvents to remove contaminants and interfering chemicals from the sample matrix and to increase the concentration of the target chemical. One expert told us that initial sample screening could benefit from reducing the number of steps in sample preparation. Furthermore, many instruments currently require pre-screening and sample preparation to operate effectively, and chemicals present in low concentrations may only be detectable after preparation.

= Near term   = Longer term

Source: Pakhnyushchyy/stock.adobe.com (background image); GAO (icons). | GAO-23-105439



Vignette

INSTRUMENTAL ANALYSIS

Analytical instruments for identifying chemical agents are mature but have a few limitations

What is it?

Analytical instruments produce information from a sample and enable investigators to identify chemical signatures which can inform attribution to a likely source. Data from instrumental analysis can also be used to build or develop new technologies.

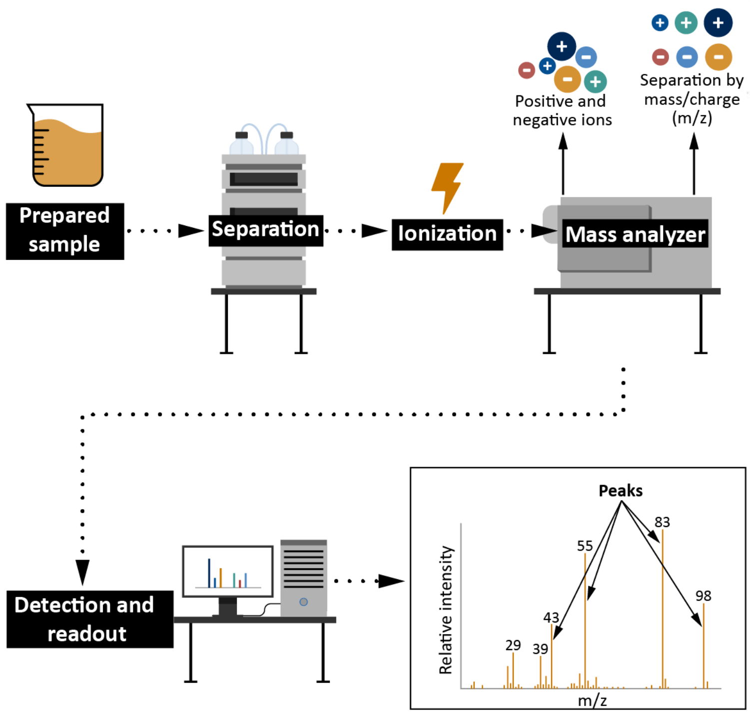
How does it work?

Instruments produce information from a sample in a variety of ways and generate a variety of information. For example, a gas or liquid chromatograph separates chemicals from a mixture and determines how much of each chemical is present. Infrared (IR), Raman, and nuclear magnetic resonance (NMR) spectrometers measure how a sample interacts with various wave forms of energy, revealing the arrangements of atoms. Mass spectrometers give an electrical charge to a molecule via ionization and then measure the mass-to-charge ratios of the resulting ions. Researchers develop methods for each instrument to analyze samples, and select appropriate methods and instruments to obtain the data they need. (For additional information on key technologies, see app. III.)

Source: GAO (header); Pakhnyushchyy/stock.adobe.com (background image). | GAO-23-105439

Real-world samples are diverse and complex, and can require initial analyses or screening to identify which preparation methods and instrumental analyses might produce the most comprehensive and accurate information. In some cases, such as OPCW investigations, chemical identifications are confirmed with one or more additional types of instruments as long as the amount of sample is large enough. The figure below shows how a prepared sample is analyzed with specialized instruments to produce chemical data.

Prepared samples are analyzed by an LC/MS instrument, one type of instrument, producing data



Source: GAO analysis of peer reviewed journal articles. | GAO-23-105439

Key Challenges

Limit of detection: Each instrument and analytical method has a specific limit of detection, below which the instrument cannot reliably detect a chemical. There are approaches to lower (i.e., improve) these limits of detection. For example, an instrument can run a method to target a specific chemical of interest, thereby reducing the limit of detection. The limit of detection is also directly related to the quantity and concentration of a sample.

INSTRUMENTAL ANALYSIS

Key Challenges *(continued)*

- **Resolution:** Instrument resolution is the ability to distinguish between signals of similar value. Every instrument has an inherent resolution, and low resolution can cause difficulty when analyzing samples containing hundreds or thousands of trace chemicals. Newer methods, such as high-resolution mass spectrometry (HRMS), may help address this challenge. But they also generate larger volumes of data than lower-resolution methods. These larger volumes of data may require advanced data analysis tools to assist investigators.

- **Sample size:** Small samples can limit the amount of data that can be generated. One reason is that investigators may need more than one instrument to gather data about different chemicals in a sample, but samples may be too small to divide for multiple analyses. Another reason is that samples prepared for one instrument may not be compatible with other instruments. For example, some instruments require samples that have undergone careful separations and modifications to remove impurities. These processes may consume precious amounts of sample, potentially introduce interferences, and reduce the information obtainable from the sample that another instrument might be able to detect.

- **Infrastructure requirements:** Instruments vary in their requirements for power, environmental controls, and data management systems, among other things. These requirements can limit the instruments' appropriateness for a given setting.

- **Workforce:** Scientists need specialized skills to operate instruments, develop analysis methods, and interpret the results. In addition, most laboratories conducting chemical agent analyses have personnel security clearance requirements and safety trainings that can take multiple years to complete.

Future Prospects

Recent incremental improvements: Incremental improvements to methods and instruments have and will continue to lower instrumental limits of detection and increase resolution. HRMS is a newer instrument type that provides high mass accuracy, resolution, and selectivity, and can further confirm the identity of potential chemical agents detected in initial screening of samples. Similarly, recent advances in chromatography, such as multiple separation steps, can provide better separation of complex mixtures.

New instrumentation developed in other fields: Experts told us that chemical forensics is a small field without the purchasing power to drive instrument development, and therefore forensic laboratories have to adapt to instruments that may be designed with other fields in mind. Other fields with more robust research and development support and larger user bases, such as the pharmaceutical industry, have analytical needs similar to the field of forensic chemical analysis. Developmental needs in these fields often result in advances in instrumentation, which experts told us have benefitted and will continue to benefit chemical forensics.

= Near term   = Longer term

Source: Pakhnyushchyy/stock.adobe.com (background image); GAO (icons). | GAO-23-105439

Vignette

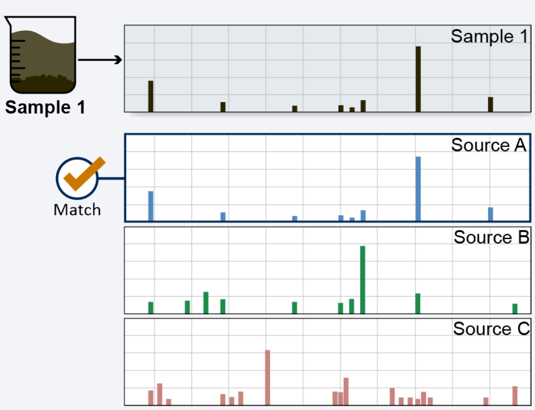
DATA INTERPRETATION

Data interpretation draws on databases of hundreds of thousands of chemicals, although these have limitations

What is it?

After an analytical instrument generates data from a chemical sample, investigators compare the data to reference data to identify the chemical or certain characteristics for attribution purposes. To do so, investigators must have access to one or more reference databases that contain data from chemicals of interest. The reference data must come from instruments with similar capabilities running a similar method.

Sample data are compared against reference data to identify a match



Source: GAO (header); GAO (figure); Pakhnyushchyy/stock.adobe.com (background image). | GAO-23-105439

How does it work?

Once investigators have data for a chemical or mixture of interest, they search for matching data in a reference library. Software often provides statistical measures of how closely the sample data and reference data match. Investigators can increase their confidence by comparing data on the same compound analyzed by multiple types of instruments.

Many entities maintain various reference libraries as a basis for chemistry research, including forensic investigations (see table). For example, the National Institute of Standards and Technology/Environmental Protection Agency/National Institutes of Health reference library contains data on more than 300,000 chemical compounds. Scientists continue to add data to this and other reference libraries.

Table 1: Three categories of reference library

Type	Purpose	Sources
General purpose data libraries	Identify known chemicals using common instruments	NIST/EPA/NIH Commercial publishers
Specialized data libraries of chemical agents and associated chemicals	Identify known chemical agents, their precursors, or associated compounds using standard or specialized instruments	OPCW – sensitive Sponsor – sensitive or classified Laboratory – internal, sensitive, or classified
Reference standard library	A physical collection of reference chemicals is used to confirm structure and formula of a compound through direct comparison; may contain information from very specific samples; and can be used to identify compounds not present in data libraries	Commercial or government chemical suppliers In-house synthesis and measurement

Source: GAO analysis of government and commercial information. | GAO-23-105439

When investigators want additional confidence in their experimental results, they can compare their experimental data to data from a sample of known makeup and purity, known as a *reference standard*. Reference standards are also needed to confidently quantify the amount of a chemical in a sample. Some reference standards—including chemical agent reference standards—can be purchased, and others are prepared by a forensic laboratory.

DATA INTERPRETATION

Key Challenges

- **Lack of data for emerging threats:** Reference data may not be available for some new chemical agents because their molecular structures and formulas are unknown by investigators.

- **Reference data may be instrument- or laboratory-specific:** Some instruments and methods may generate unique data that do not match data in accessible reference libraries. In those cases, scientists may need to build a reference library that is specific to that instrument. Experts told us laboratories are reluctant to share their in-house reference libraries or data due to concerns about data sensitivity and competitive advantage. For example, if a laboratory shares in-house reference data for a chemical agent, a bad actor may use that information to make a sample of the same agent that produces similar laboratory results.

- **Reference libraries for hand-held instrumentation are limited:** One expert told us that built-in libraries for handheld instruments are limited.

- **Data from improved instrumentation require more computing power and can hinder database matching:** As improvements in instrumentation provide higher-resolution data and lower limits of detection, processing those data requires increased computing power. In addition, experts told us that modern instrumentation may discern signals that previously were not detectable, which can complicate database matching.

- **Authentic reference chemicals can degrade:** Reference standards, which investigators use when they need to verify the presence of a chemical in a sample or provide quantitative results, can degrade over time and may need to be produced on an as-needed basis by chemists.

Future Prospects

Computational prediction: Researchers have begun training machine-learning-based computational methods to predict characteristics of chemicals on the basis of their structure. Use of these systems could fill data gaps in reference libraries and help identify unknown compounds.

Analytical methods that are less reliant on reference data: Improvements in mass spectrometry (MS) instruments, such as HRMS, may provide higher-precision data and reduce reliance on reference data.

Universal ionization: Experts suggested development of universal ionization—a MS ionization technology that works with both gas chromatography (GC) and liquid chromatography (LC) systems. GC-MS and LC-MS data are currently not comparable, but universal ionization could make comparison possible.

= Near term   = Longer term

Source: Pakhnyushchyy/stock.adobe.com (background image); GAO (icons). | GAO-23-105439

2.2 Methods for attributing chemical agents based on chemical analyses are under development

Researchers are developing methods that could attribute a chemical agent to its likely source based on chemical analyses. Such technologies could reduce reliance on other types of forensic evidence if other factors align, such as access to the right reference data. However, such data are limited and typically different from the reference data needed to identify a chemical agent.

Two key technologies show promise for this purpose: *impurity profiling* and *isotope ratio methods*. Both methods identify specific chemical information about precursor chemicals made by different manufacturers. Both methods may rely on access to, measurement of, and comparison against precursors.

Impurity profiling identifies and measures impurities that are present in existing samples of chemical agents or known precursor supplies and compares those with impurities in incident samples.[13]

- **Benefits:** A match between the impurities present in an incident sample and those in a known precursor supply can increase investigators' confidence that a chemical agent was made from that supply. It can also give clues about the synthetic route used to make a chemical agent.
- **Status:** Impurity profiling has been used in some real-world cases, including the United Nations/OPCW investigation into sarin attacks in Khan Shaykoun, Syria. However, more research is necessary for broader operational use of this technique.
- **Limitations:** When dispersed in a matrix, impurity levels may be below the limit of detection. In addition, impurities are not necessarily stable over time, so direct comparisons may be difficult as a sample degrades. For example, OPCW investigators conducted impurity profiling on two samples of Novichok agent used in an assassination attempt in the United Kingdom. However, because one sample was exposed to the environment and the other was not, the investigators in this case were unable to determine whether the samples were from the same source.

Key concept: A ***chemical surrogate*** is a chemical used to mimic the properties of a chemical agent but reduce the risk posed by handling the material. Chemical surrogates are used by researchers to develop and evaluate methods that may be useful with chemical agents. These chemicals do not have the same restrictions and risks as chemical agents and can be used in general laboratories that are not certified chemical surety laboratories.

Source: GAO analysis of information from an expert and scientific literature. | GAO-22-105439

[13]The instrumentation used for impurity profiling includes GC, LC, MS, and NMR.

Isotope ratio methods use specific instrumentation to measure the ratio of isotopes of certain elements in samples to determine the *isotopic signature* of the material.[14]

- **Benefits:** It may be possible to use isotope ratio data to link degradation products directly to precursor data or samples.
- **Status:** These methods have been established and used for years in many applications, including archeology and geochemistry. Their application to attribution of chemical agent precursors and surrogates has been described in peer-reviewed literature in the past decade. However, more research is necessary for broader operational use of this technique.
- **Limitations**: In some cases, these methods require relatively pure samples of precursors or the agent itself for direct comparison to an incident sample. These methods could also be less effective for some complex samples where the chemical agent is dispersed in a matrix. Further, for these methods to be successful, additional information may be needed about the synthetic route that was used.

In addition to impurity profiling and isotope ratio methods, researchers have been working to develop and improve machine learning algorithms to help investigators determine the synthetic route used to make a sample. These methods apply statistical and mathematical models to detect patterns in data from complex samples using pattern recognition algorithms trained on historical data. However, they rely on training the algorithms with appropriate data. As a result, they may not perform well on emerging threats for which data are limited, such as on chemical agents made using unreported synthetic routes, or on samples in complex matrices.

Even when the technologies and methods described above can match a chemical to an existing sample, certain circumstances can hinder attribution. For example, some mass-produced chemicals, such as certain pharmaceuticals and toxic industrial materials, can be weaponized. These chemicals can be much harder to attribute because many producers obtain raw materials from common sources, which may trace back to geographical locations far from the manufacturing site.

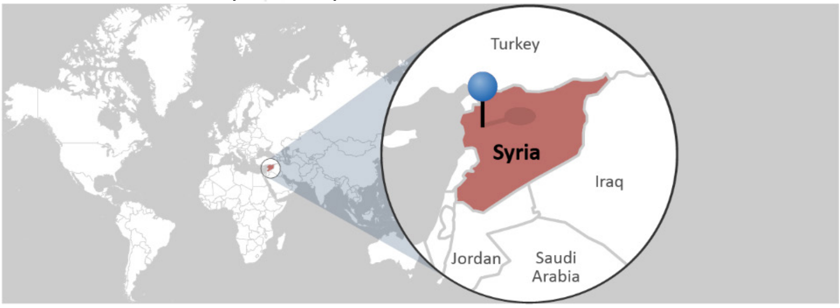
[14]Isotopes are atoms of the same element that have different atomic mass. Materials from different sources may differ in the ratios of isotopes they contain, and this difference may therefore be useful in distinguishing sources. The instrumentation used for isotope ratio methods includes MS and NMR. NMR is earlier in development for isotope ratio analyses than MS.

2.3 Real Event Summaries

In this section we will provide summaries into publicly-reported forensic investigations conducted by the OPCW after two chemical incidents in Syria and two in the United Kingdom. These summaries provide context about the event, the chemical agents involved, technologies used to identify and attribute the chemical agent, and specific challenges faced by investigators during those investigations. We will discuss these challenges in greater depth, along with others, in chapter 3.

KHAN SHAYKHUN CHEMICAL INCIDENT

Location: Khan Shaykhun, Syria



Sources: GAO analysis of OPCW reports; Map Resources (map). | GAO-23-105439

Date: April 4, 2017

Chemical type: Nerve agent (sarin)

Scenario: Internal conflict

Event: During an internal conflict in Syria, an aerial chemical weapon attack in the town of Khan Shaykhun exposed approximately 292 people to sarin or a sarin-like substance, resulting in 50 fatalities.

Technologies used: Gas chromatography-mass spectrometry and impurity profiling.

Challenges:

- Delayed access to the incident site due to lack of permission and security concerns.
- Disturbance of the site limited the variety of evidence collected.

April 5 - June 22 2017, OPCW Fact Finding Mission (FFM): [15]

Investigators obtained statements, documents, photos, and videos from witnesses. Witnesses also gave investigators dead birds, hair from a dead goat, clothes, vegetation, rock, and soil samples. Investigators obtained blood and urine from 10 casualties.

The mission concluded that a large number of people were exposed to sarin or a sarin-like substance.

June 23 - October 25 2017, OPCW-United Nations-Joint Investigative Mechanism (JIM): [16]

The JIM used the following forensic chemistry techniques in their investigation of the Khan Shaykhun sarin attacks:

- Synthetic route identification: Confirmed that sarin was produced by a specific synthetic route in which a sarin precursor, methylphosphonyl difluoride (DF), was combined with isopropyl alcohol in the presence of hexamine.
- Impurity profiling: Identified an impurity, phosphorus hexafluoride (PF6), in all environmental samples.
- Reference data: OPCW had DF from Syrian chemical weapons stockpiles collected in 2014. Laboratory analyses of these reference samples confirmed the presence of PF6.

The JIM concluded that the presence of PF6 was evidence of the process used to produce the sarin precursor DF. The JIM further concluded that sarin identified in the samples taken from Khan Shaykhun was most likely made with a precursor (DF) from the original Syrian stockpile.

All-source analysis of Khan Shaykhun incident:

The JIM assembled a detailed timeline of the incident, along with photographs, videos and satellite images, and crater and munition analysis, among other things. On the basis of these observations, along with the sudden high number of casualties, the FFM and JIM concluded that the evidence pointed to the deliberate release of a toxic chemical.

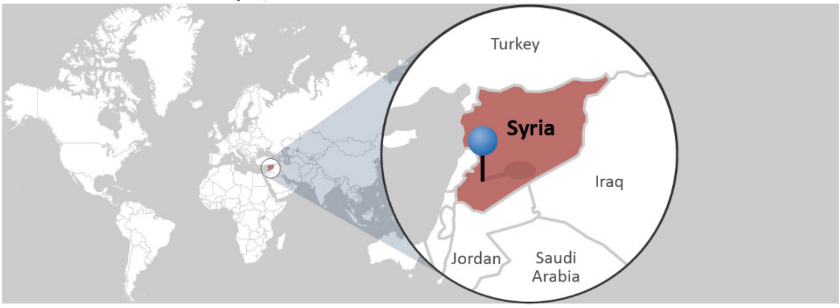
Sources: GAO analysis of OPCW reports; Pakhnyushchyy/stock.adobe.com (background); GAO (icons). | GAO-23-105439

[15] Note by the OPCW Technical Secretariat, "Report of the OPCW Fact-Finding Mission in Syria Regarding an Alleged incident in Khan Shaykhun, Syrian Arab Republic, April 2017," S/2017/567.

[16] "Seventh report of the Organisation for the Prohibition of Chemical Weapons - United Nations Joint Investigative Mechanism," S/2017/904.

DOUMA CHEMICAL INCIDENT

Location: Douma, Syria



Sources: GAO analysis of OPCW reports; Map Resources (map). | GAO-23-105439

Date: April 7, 2018

Chemical type: Chlorine

Scenario: Internal conflict

Event: During fighting in the city of Douma, Syria, two gas cylinders were dropped on residential buildings and released their contents, killing 43 individuals and injuring dozens more.

Technologies used: LC-HRMS and NMR.

Challenges faced by the OPCW Fact Finding Mission (FFM) team and Investigation and Identification Team (IIT):

- Inability to access site in a timely manner due to lack of permission and high security risks.
- Difficulties in gathering information and lack of cooperation from the Syrian Arab Republic.

March 1, 2019: Report by OPCW FFM:[17]

- Evidence gathering, sample collection, and detection: The FFM team collected environmental samples and detected chlorinated organic chemicals—which are not naturally present—in several samples.
- Identification: The FFM team was able to confirm that objects had been in contact with 'reactive chlorine'.

January 27, 2023: Report by OPCW IIT:[18]

- Detection and analyses: The IIT confirmed the presence of highly chlorinated phenols in samples collected, indicating the release of chlorine gas at high concentrations. Furthermore, the symptoms of the victims were consistent with exposure to chlorine gas in very high concentrations leading to a high fatality rate.
- Dispersion modeling: Two independent gas dispersion models considered by the IIT indicated that fatalities were a result of exposure to a rapid release of chlorine gas.

All-source analysis of Douma incident and source attribution:

- The FFM's all-source review included witness testimonies, environmental and biomedical analysis results, toxicological and ballistic analyses from experts, and videos and images from witnesses. The IIT was able to rule out other hypothesis such as the possibility of a staged incident.
- The IIT concluded that at least one helicopter of the Syrian Arab Air Force dropped two cylinders containing chlorine, one of which hit a residential building, ruptured, and rapidly released toxic chlorine gas in very high concentrations, which dispersed within the building killing 43 individuals and affecting dozens more.

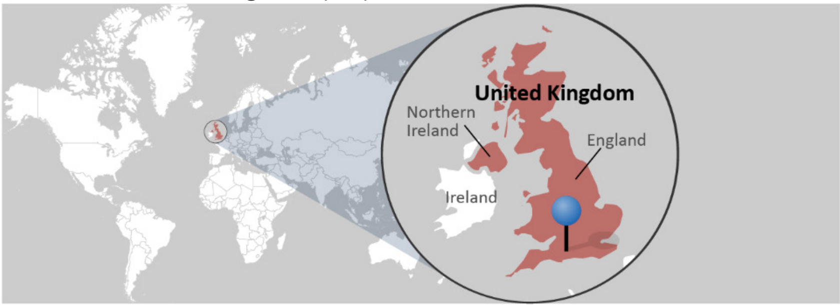
Sources: GAO analysis of OPCW reports; Pakhnyushchyy/stock.adobe.com (background); GAO (icons). | GAO-23-105439

[17] Note by the OPCW Technical Secretariat, "Report of the Fact-Finding Mission Regarding the Incident of Alleged Use of Toxic Chemicals as a Weapon in Douma, Syrian Arab Republic, on 7 April 2018," S/1731/2019 (2019).

[18] Note by the OPCW Technical Secretariat, "Third Report by the OPCW Investigation and Identification Team Pursuant to Paragraph 10 of Decision C-SS-4/Dec.3 "Addressing the Threat from Chemical Weapons Use" Douma (Syrian Arab Republic)-7 April 2018," S/2125/2023 (2023).

SALISBURY AND AMESBURY CHEMICAL INCIDENTS

Location: United Kingdom (UK)



Sources: GAO analysis of OPCW reports; Map Resources (map). | GAO-23-105439

Date: March – June 2018

Chemical type: Nerve agent (Novichok)

Scenario: Assassination attempt

Event: Two people—a British citizen and his Russian citizen daughter—in Salisbury, United Kingdom (UK), were poisoned by a nerve agent on a doorknob; both individuals survived. Months later, two other individuals were exposed to a similar nerve agent contained in a glass jar in Amesbury, UK; one died.

Technologies used: Impurity profiling (inconclusive), others not reported.

Challenges:

- Unknown sample storage conditions and degradation.

March – April 2018, Salisbury, UK, OPCW Response to Technical Assistance Request: [19]

British authorities identified and publicly announced the substance as a Novichok, an advanced nerve agent originally developed in the Soviet Union. OPCW investigators obtained information including victim status and treatment, blood samples, environmental samples, and part of the samples collected by British authorities (known as split samples).

Based on this evidence, the OPCW's analysis demonstrated the presence of a nerve agent and confirmed the UK's identification of the nerve agent. OPCW's analysis also determined the nerve agent was of a high purity.

June – September 2018, Amesbury, UK, OPCW Response to Technical Assistance Request: [20]

OPCW obtained victim status and treatment information, blood samples, biomedical samples, environmental samples, and biomedical split samples taken by British authorities. OPCW later collected blood samples, attended and observed the autopsy of one victim, and collected a sample from a small bottle that the police seized from the incident site.

OPCW's analysis demonstrated that the two victims were exposed to and affected by the nerve agent. The analysis also showed that the sample consisted of a highly concentrated nerve agent that was 97 to 98 percent pure. OPCW confirmed the UK's identification of the nerve agent and confirmed that it was the same agent found in the Salisbury incident samples. OPCW could not conclude whether the samples from the Salisbury and Amesbury incidents were from the same synthesis batch because of unknown storage conditions and degradation.

Sources: GAO analysis of OPCW reports; Pakhnyushchyy/stock.adobe.com (background); GAO (icons). | GAO-23-105439

[19] Note by the OPCW Technical Secretariat, "Summary of the Report on Activities Carried out in Support of a request for Technical Assistance by the United Kingdom of Great Britain and Northern Ireland (Technical Assistance Visit TAV/02/18)," S/1612/2018 April (2018).

[20] Note by the OPCW Technical Secretariat, "Summary of the Report on Activities Carried out in Support of a Request for Technical Assistance by the United Kingdom of Great Britain and Northern Ireland, (Technical Assistance Visit TAV/03/18 and TAV/03B/18, Amesbury Incident," S/1671/2018 September (2018).

3 Several Challenges Can Hinder Identification of Chemical Agents and Their Sources

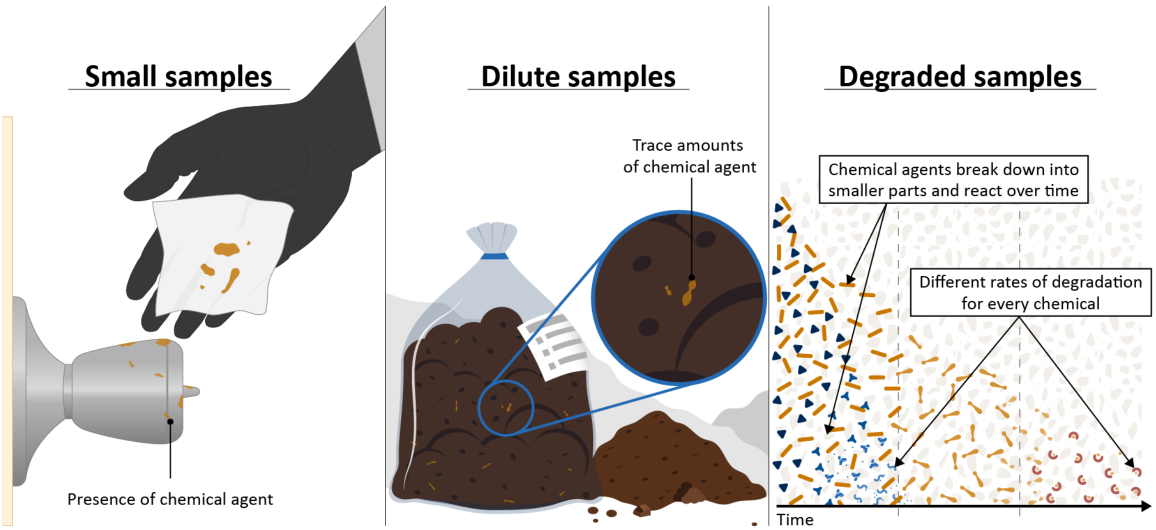
We found that several challenges can hinder identification of chemical agents and their likely sources. First, samples can be too small or degraded for analyses to provide useful chemical information. Second, limited or incompatible reference data may lead to inconclusive results. Third, the sensitive nature of some information on chemical agents and methods may complicate collaboration and information sharing that could advance the field. And fourth, many entities support chemical agent forensics, but coordination is limited.

3.1 Small, dilute, or degraded samples can reduce the utility of chemical analysis

When high-quality samples are not available, chemical analysis can be challenging (see fig. 2). Small samples—such as one collected on a single cotton swab—pose a particular challenge because scientists may have difficulty splitting the sample to perform multiple tests—a measure that can provide a higher degree of confidence in the results.[21] Similarly, in samples containing only trace amounts of a chemical agent, the agent can be masked by or react with other chemicals, or its concentration may be below the instrument's limit of detection. A degraded sample can also be challenging to analyze because degradation products can be numerous, and reference data are often limited.

[21]While investigators may have difficulty splitting small samples, some retain enough material for analysis.

Figure 4: Samples can be small, dilute, or degraded



Source: GAO. | GAO-23-105439

Investigators should ensure they try to gather high-quality samples, but the circumstances do not always allow for this. We identified three categories of challenges that can result in small or degraded samples:

- **Site access**. The time it takes investigators to access an incident site depends on a variety of factors, including location of the incident, time of the incident, and/or distance from the incident site to the nearest capable response team. For example, FBI investigators may access domestic sites of chemical incidents within hours. However, investigators for an OPCW mission in Douma, Syria, could not collect environmental samples from the site of a suspected chemical incident until 14 days after the incident because of security concerns.

  Such delays can reduce sample quality. For example, sarin quickly degrades in the environment, and some of its degradation products also evaporate quickly. On the other hand, chemical agents such as VX may persist in the environment for weeks because they are not as prone to degradation.[22]

- **Sample collection.** Even if they arrive promptly, investigators can face challenges identifying sampling locations and materials to collect once on site. For example, chemical agents like chlorine are reactive and dissipate quickly. Additionally, if chemical agents are released into the air over large areas, they may only be present at potential sampling locations in low concentrations. Incident scenes can also be disturbed. For example, the site of the alleged attack in Khan Shaykhun, Syria, was filled with concrete before investigators arrived. Experts told us that some efforts are

[22]VX is a chemical warfare agent and categorized as a nerve agent.

underway to improve future sample collection.

- **Transportation issues.** Experts told us that, in some cases and depending on the chemicals involved, delays and other issues with transportation of samples for analysis can sometimes reduce sample quality. Experts told us that transportation delays sometimes occur because of regulations and export controls, which can make it difficult to obtain permission to fly a sample through a nation's airspace. One agency official told us investigators sometimes lack cold containers or other appropriate packaging to use during transportation, which can exacerbate this issue.

3.2 Chemical reference data may be limited or incompatible

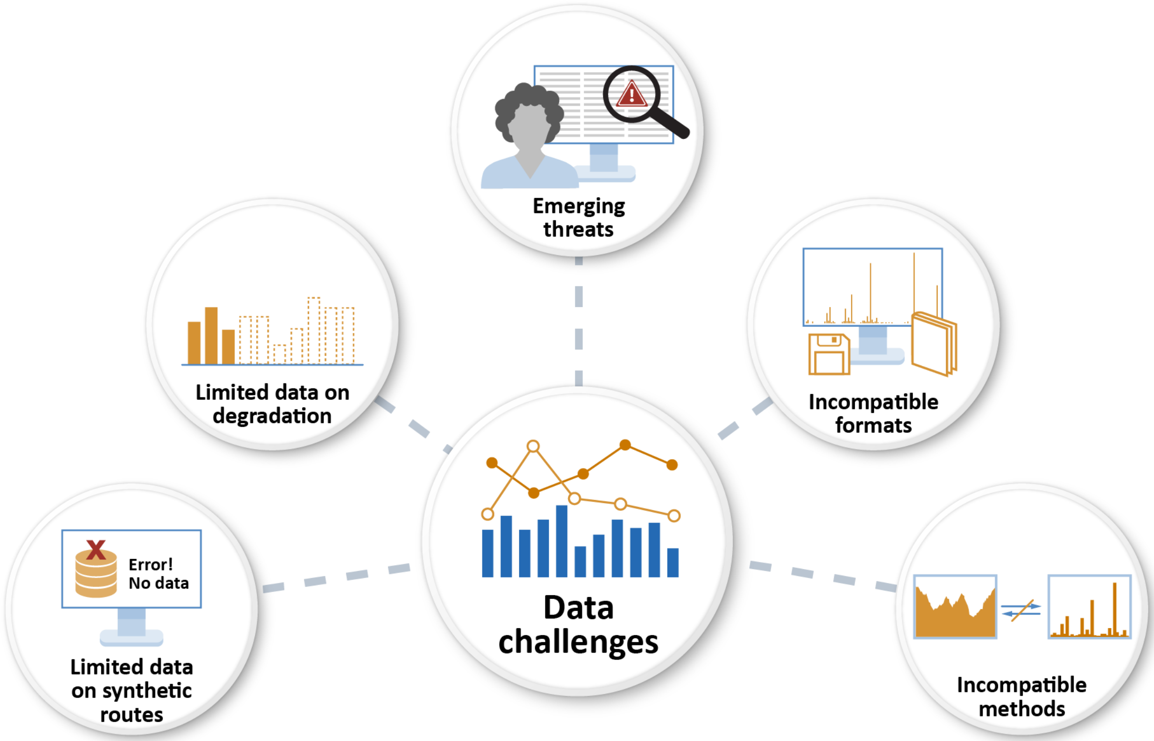
Reference data are not available for all chemical agents, which can make identification challenging.[23] One reason reference data are limited is that millions of chemicals could theoretically be used as chemical agents or to manufacture chemical agents.[24] In addition, many chemicals can be made using multiple methods, and may degrade differently depending on environmental conditions. This means that, for a given chemical agent, additional reference data may be needed.

Generally, methods used to identify chemical agents rely on comparison with reference data. Scientists compare the data from incident samples against a variety of databases that contain reference data, including commercial databases, databases maintained by sponsoring entities, or databases internal to a laboratory.

[23] One agency emphasized the importance of physical samples being available for study and measurement. This is in part because reference data are often based on physical samples. In addition, samples can sometimes be used for direct comparison with a sample from a chemical incident.

[24] Stefan Mogl, "Sampling and Analysis in the Chemical Weapons Convention and the OPCW Mobile Laboratory," in *Chemical Weapons Convention Chemicals Analysis*, ed. Markku Mesilaakso (John Wiley & Sons, Ltd, 2005), 9.

Figure 5: Types of data challenges to chemical identification and attribution



Source: GAO. | GAO-23-105439

Experts described five specific data limitations that complicate chemical agent analysis (see fig. 5):

- **Limited reference data on synthetic routes**. Reference data on the possible synthetic routes for chemical agents may help investigators determine or rule out potential sources, but these data are limited for multiple reasons. Experts told us studying the numerous ways chemical agents can be produced is time- and resource-intensive. One expert estimated that studying one chemical agent and four to six synthetic routes would require four laboratories working between 18 and 24 months.
- **Limited reference data on degradation.** Reference data on chemical agent degradation may help investigators determine a chemical agent's identity or source, but these data are limited. One reason is the variety of possible degradation routes depending on the chemical and environmental factors. Another reason is that chemical surrogates and pure chemical agent samples may not degrade in the same way as incident samples. Furthermore, certain databases do not include comprehensive data on degradation products. For example, the OPCW Central

Analytical Database does not include information on some degradation products.

Experts have differing views on the feasibility of determining the source of degraded samples. Some told us it is important to understand degradation because chemical agents can degrade quickly, and degradation products may be all that remain in some samples. However, others think it is difficult to determine the source of some degraded samples because it could require experiments with several chemical agents degrading under a range of conditions to find a match. In some instances, investigators have found it difficult to reach conclusions because of degradation. For example, as previously noted, following two chemical incidents in the United Kingdom, the OPCW could not determine whether chemical agents originated from the same synthesis batch because one of the agents had degraded.

- **Emerging threats.** A vast number of chemicals exist or are being created for a variety of purposes, and some of them could be used as chemical agents or to manufacture one. Rigorous research into emerging threats takes significant time and effort, which means reference data are sometimes unavailable. In addition, laboratory officials told us a chemical agent may be created or altered in a way such that it does not match reference data.
- **Incompatible methods.** Researchers may not be able to use some data as reference data if they were collected using different methods or instrumentation, which can limit data sharing between laboratories. For example, even data collected from similar instruments, such as two LC-MS analyses, may not be directly comparable if the experimental designs differ. In general, experts told us standardized methods and instrumentation settings can help to improve knowledge building and data comparison within and between laboratories. Without compatible data, researchers may unnecessarily duplicate experiments, and knowledge building of chemical agents may be slowed.
- **Incompatible formats.** Some reference data may be incompatible with new data because they are stored using different media and formats. Since the beginning of modern chemical agent research programs during World War I, data have often been stored in laboratory notebooks, notecards, and hard drives, and in other formats that are not readily accessible to a range of users, according to experts. In addition, modern instruments are significantly more sensitive than historical instruments. As a result, it is difficult to combine or compare previously collected data from different eras, which may limit the ability of emerging technologies—such as machine learning systems—to use historical data to predict and identify chemical threats.

3.3 The sensitive nature of chemical agent forensics poses challenges to information sharing

National security classification and sensitivity may complicate collaboration and information sharing that could help to develop technologies and improve understanding of chemical agents and their sources.[25] This information includes reference data and sample preparation methods. Many entities are involved with chemical agent forensic analysis or research that can support analysis (see Table 2). Experts told us their various sponsoring entities may have different classification guides, and that this complicates determining whether information is classified and with whom it can be shared. However, classification is important, and a significant amount of information about chemical agents is classified to protect national security.

Experts described three main areas affected by classified and sensitive information:

- **Technology development.** Agency officials told us that restrictions on information sharing may limit the involvement of private industry and academic researchers, which are key players in technology development. For example, classification sometimes limits industry enthusiasm and willingness to work on a technology because sponsoring entities cannot communicate to potential developers why they need the new technologies. Additionally, some industry and university stakeholders do not have the infrastructure to handle classified information or appropriately cleared personnel able to perform classified work.
- **Research collaboration.** Officials from one laboratory told us that it is difficult and time consuming to design international collaborations because sponsoring entities may not all agree on what is shareable. Research collaboration challenges may limit opportunities to share information and co-develop or corroborate research methods, which are important steps for knowledge building.
- **Reference data sharing and publishing.** Laboratory officials told us it can be challenging to determine what information may be shared or published, which can slow or prevent the sharing of reference data. For example, researchers are wary of sharing sensitive information because adversaries might access this information and use it to make chemical agents, or to cast doubt on an investigation's techniques and findings, among other reasons. Additionally, internal laboratory databases are not broadly shared because of concerns about sensitivity and sharing proprietary information, according to experts and agency officials. Officials from one laboratory told us some sponsoring entities also discourage publishing research publicly. This lack of shared reference data could result in researchers unknowingly duplicating experiments or lacking awareness of each other's work, which could limit scientific advances and overall chemical forensic analysis capabilities.

[25]We define sensitive information as information that could adversely affect national interest or conduct of federal programs, but that has not been specifically authorized under criteria established by an Executive Order or an Act of Congress to be kept classified in the interest of national defense or foreign policy.

3.4 Limited coordination hinders improvements to methods and technology

Another challenge to the identification of chemical agents and their sources is limited coordination among entities that use and develop chemical forensic technologies. Multiple experts told us there is limited coordination among entities using the technologies and that no central authority facilitates information sharing. Instead, information about such entities' use of chemical forensics is siloed, according to agency officials. For example, Department of Defense officials told us that the Defense Intelligence Agency; U.S. Central Command; U.S. Special Operations Command; and the 20th Chemical, Biological, Radiological, Nuclear, and Explosives Command use different data systems to track chemical agent samples they collect. Under these circumstances, each unit may expend resources to collect and analyze a sample that another unit has already analyzed. However, sponsoring entities expressed differing views about the utility of splitting incident samples for analysis by multiple laboratories.

Coordination is also limited among sponsoring entities and the research community. For example, some non-surety laboratories use surrogate chemicals or limited quantities of chemical agents to develop methods that could inform attribution. Experts told us that the transfer of knowledge from these laboratories to surety laboratories requires more coordination. Additionally, some sponsoring entities do not allow laboratories to share methods developed for the sponsor's work. Experts told us this could result in unnecessarily duplicative work developing new methods to analyze samples when researchers could use existing methods.

One reason for the limited coordination is that each sponsoring entity has its own specific goals, requirements, and capabilities. For example, officials from the Army 20th Chemical, Biological, Radiological, Nuclear, and Explosives Command told us they conduct chemical analysis for identification but not for attribution, since their key goal is to understand battlefield conditions and ensure troop protection. By contrast, other entities have different goals, which include attributing chemical attacks to specific sources.

Another reason for the limited coordination is that some of the current funding approaches for the laboratories can restrict research collaboration as well as research that might be broadly useful. Sponsoring entities provide laboratories with funding, and laboratories compete for resources from the sponsoring entities. Officials from one laboratory said they primarily receive funding—using a reimbursement approach—to analyze specific samples for sponsoring entities. They are not funded to conduct forensic research on chemical agents, or other research that might be of wider benefit. For example, they are not generally funded to identify and aggregate legacy data that might provide a useful source of reference data. Some other laboratory officials told us they have funding arrangements with sponsoring entities that allow research, providing more flexibility in their work. However, both funding arrangements may make laboratories reluctant to share information with each other, for fear that it will help other laboratories compete for funding. DOD officials noted that coordination between sponsoring entities can facilitate sharing of information.

The result of this limited coordination is that researchers are not always aware of each other’s work, and they may unknowingly duplicate work or miss opportunities to strengthen their capabilities through cooperation. Furthermore, laboratories and sponsoring entities may not be aware of expertise that could assist with identifying a chemical agent or its source. And sponsoring entities may not coordinate to develop or procure new technologies, potentially missing opportunities to drive technology development with their combined purchasing power.

Some experts and officials we met with expressed interest in working more closely with other laboratories to share and develop methods. This collaboration can be especially important for emerging techniques because it can increase confidence in those techniques. Laboratory officials explained that splitting samples and having multiple laboratories testing one another’s methods can increase confidence in results.

4 Six Policy Options to Help Address the Challenges that Hinder Identification and Attribution of Chemical Agents and Their Sources

As discussed in chapter 3, we identified the following key challenges to identification and attribution of chemical agents and their sources:

- Small, dilute, or degraded samples can reduce the utility of chemical analysis.
- Chemical reference data may be limited or incompatible.
- The sensitive nature of chemical agent forensics poses challenges to information sharing.
- Limited coordination hinders improvements to methods and technologies.

We identified six policy options that policymakers could consider in response to these challenges. These policymakers include Congress, federal agencies, state and local governments, academic and research institutions, and industry. For each policy option, we present potential implementation approaches, some of which specify a policymaker based on the approach. This is not an exhaustive list of policy options. We present them to assist policymakers who aim to further advance chemical agent identification and attribution technologies.

Policy option: Policymakers could encourage development of technologies that allow more rapid sample analysis or that slow sample degradation

Challenge addressed: Small, dilute, or degraded samples can reduce the utility of chemical analysis.

Potential implementation approaches

- Identify opportunities for partnering in research fields with similar technical requirements to develop more capable field-deployable instrumentation and sampling technologies. For example, drones could be developed to collect and transport chemical agent samples with less risk to personnel.
- Encourage cross-agency partnering on technology research, development, and procurement to leverage buying power. With greater buying power, agencies could better incentivize industry to develop technologies that inform attribution, such as detection tools that could rapidly provide information in the field.
- Federal agencies could develop an interagency strategic plan for forensic technology development and acquisition. A strategic plan allows the federal government to communicate its current and future needs to companies and researchers, which could then align their internal research and development to the government's needs.

Opportunities

- The development of instrumentation that could enable more effective analysis in the field would reduce the time between sampling and analysis. It could also reduce degradation in some cases, potentially improving the reliability of some analyses and enabling faster decision-making.

- Faster information delivery to decision-makers could enable more rapid treatment, countermeasure deployment, and military or diplomatic actions.
- Rapid collection and analysis of samples may reduce the investment needed by minimizing the number of chemical signatures generated by sample degradation.

Considerations

- Small market size for certain instrumentation and barriers to entry for classified work may limit industry interest in developing new technology. Barriers to entry for classified work include obtaining appropriate clearances for personnel and building out a physical space that can be used for classified work.
- New technologies require testing and evaluation to ensure they function properly in real-world conditions. This likely requires more funding and time in the case of chemical agents due to their toxicity and reactivity.

Policy option: Policymakers could advance scientific knowledge on known chemical agents and threats

Challenge addressed: Chemical reference data may be limited or incompatible.

Potential implementation approaches

- Support experimental research on known chemical agents and threats to expand fundamental understanding of their synthetic routes and degradation pathways. One expert told us that this type of work is complex, time consuming, and currently underfunded, but could lead to more robust data on chemical agents and threats. For example, data could be gathered from months-long experiments looking at how chemical agents and threats degrade in different matrices, such as sand versus clay soil, and react to different pollutants.
- Increase support to research into computational approaches to fill gaps in existing knowledge. Computational approaches extrapolate chemical information from known samples to create data for chemicals that have not been sampled. This could allow for more complete data without access to certain samples, though data from computational extrapolation may have greater uncertainty.
- Federal agencies could develop long-term interagency research plans that coordinate efforts to expand and fill gaps in knowledge of known chemical threats. This type of plan could specify how data and methods from research are to be shared across the government, giving agencies access to additional research data and methods.

Opportunities

- Improved ability to identify known chemicals could support a faster response to an event, and faster attribution.

- Sustained support of research could ensure that the U.S. has the appropriate workforces, capabilities, knowledge, and facilities to respond effectively to threats.
- Coordination of research efforts may leverage information more effectively and prevent duplication.

Considerations

- In some cases, additional knowledge may not enable the identification or attribution of a chemical to its source due to highly degraded samples or chemicals intentionally created to not match reference data. Additionally, one expert told us that the number of synthetic routes for a chemical agent can be so large that research in the area may not be practical.
- Building the necessary body of knowledge could be time and resource-intensive.

Policy option: Federal policymakers could foster development of technologies and approaches that help anticipate emerging chemical threats

Challenge addressed: Chemical reference data may be limited or incompatible.

Potential implementation approaches

- Support development of technologies focused on detecting and characterizing emerging chemical threats for which reference data or standards may not be available. For example, one expert told us emerging research might make it possible to deduce chemical information without an exact reference sample. Researchers could use similar samples and advanced computational approaches to model chemical information on an unknown chemical agent.
- Support research into computational approaches to identify and predict properties of emerging chemical threats.

Opportunities

- Identification of emerging chemical threats could deter use and support a faster response in the event of use.
- Emerging chemical threat assessment and characterization technologies could better prepare U.S. government entities and international partners for the unexpected.

Considerations

- A vast number of chemicals and some precursors are emerging chemical threats, and efforts would require careful prioritization. This could be difficult as different entities may have competing priorities.
- Computational approaches designed to identify a vast number of potential compounds would require security considerations to protect previously or potentially classified chemicals.

Policy option: Policymakers could encourage standardization of future data collection and support efforts to modernize legacy data on chemical threats

Challenge addressed: Chemical reference data may be limited or incompatible.

Potential implementation approaches

- Expand existing international efforts to develop standards for reporting out the results of chemical forensic analyses. For example, one expert told us there is a need for standardized format of data generated in a chemical forensic analysis.
- Initiate efforts to assess legacy data stored in diverse formats and convert them into modern formats that could be easily read by artificial intelligence and machine learning methods. For example, Department of Defense laboratory officials told us they have some data stored in notebooks, which would need to be digitized to become machine readable. In another example, one expert suggested a multiyear effort specifically to consolidate data from literature into a usable database. One agency noted that database consolidation has been attempted in the past, and that a useful first step within the US Government would be to identify all existing US Government databases and assess their applicability for such an effort.

Opportunities

- Standardization could ensure that predictive and machine learning computational methods may be applied to data collected by different sources, maximizing potential insights and resources. For example, there are many different libraries of reference data on chemical agents, and machine learning could be used to compare and combine them.
- Researchers may be able to use modernized legacy data to gain insights that are otherwise expensive or difficult to acquire. For example, legacy data were collected during offensive chemical weapons programs, which have since ended.

Considerations

- Some legacy data have been collected using different experimental design, instrumentation, and analytical techniques than those currently used. As a result, the data may be more challenging to use in certain circumstances. Additionally, any sensitivities or classification concerns would need to be addressed before data could be made available.
- Efforts to identify and aggregate useful legacy data can be difficult and time consuming and are rarely funded by sponsors.
- Consensus on standard operating procedures may be difficult to achieve.

Policy option: Federal and international policymakers could facilitate information sharing to increase collaboration on chemical agent forensic analyses

Challenge addressed: The sensitive nature of chemical agent forensics poses challenges to information sharing.

Potential implementation approaches

- Agencies could create or update security classification guides to consult with laboratory researchers for input on areas where classification guides may cause confusion or appear to be contradictory.

- Agencies with classification guides in this area could consider communicating with each other when creating or updating classification guides to facilitate consistency and uniformity of classification decisions.[26]
- Support development of mechanisms to quickly determine the classification level for new information on chemical threats. Agency officials told us that routine classification updates are not fast enough for the pace of change of emerging chemical threats.
- Support development of training or tools that help research and development entities navigate complex classification scenarios. For example, agencies could distill complicated classification guidance into more user-friendly decision aids for staff.
- For both a whole-of-government approach and within agencies, facilitate communication between appropriately cleared personnel to understand: 1) where parallel or complementary research and development efforts may be ongoing and 2) locations of relevant expertise or data. For example, formal agreements between entities could clarify what information can be shared.

Opportunities

- Quickly making classification decisions about new and emerging information could improve appropriate domestic and international research collaboration and information exchange.
- Information and expertise sharing between entities could improve capabilities and reduce duplicative, resource-intensive experimentation.
- Data sharing between entities could provide new insights, such as through the use of data science tools to examine combined data sets.
- Increased understanding of classification guidance could improve handling of classified information and allow researchers to more confidently know what information can be shared.

Considerations

- Agencies with classification authorities may be reluctant to take steps that could lessen individual agency control over classified information.
- Classification systems are complex and creating tools to assist in navigating them could be challenging.
- Agencies need to balance facilitating additional information sharing with protecting information critical to national security.

[26] 32 C.F.R. §2001.15(a) encourages originators of classification guides to consult with end users and, when possible, communicate with other agencies when developing classification guides.

Policy option: Federal and international policymakers could encourage increased coordination between entities involved in chemical attribution

Challenge addressed: Limited coordination hinders improvements to methods and technologies.

Potential implementation approaches

- Encourage entities that fund laboratories to coordinate on the sharing of methods, equipment, and results to reduce duplication of work and increase knowledge sharing.
- As a whole-of-government approach, identify roles and responsibilities of agencies and gaps in the current structure. For example, in the related area of biological threats, the White House created the National Biodefense Strategy and related policy to coordinate federal biodefense activities to enhance capabilities for forensics and attribution of biological threats.[27]
- Encourage interagency and international cross government exercises to improve coordination and execution of chemical forensics. For example, agencies could develop a concept of operations for all the steps in chemical forensic analysis.
- To better understand laboratory capabilities and expertise related to chemical attribution, encourage collaboration between international partners, such as those involved with the Chemical Forensics International Technical Working Group. For example, that group could institute new confidence-building exercises.[28] In these exercises, laboratories could independently attribute a number of samples to a likely source using both OPCW suggested methods and the laboratory's own methods, and then compare results.

Opportunities

- Better coordination between U.S. government agencies could change the culture so information sharing becomes the normal mode of operation.
- Breaking down silos of information at different levels across government would allow entities to better collaborate and share legacy data, new methods, and research findings.
- Identifying clear roles and responsibilities enables each entity to quickly execute its mission in response to a chemical incident.
- Collective development of robust methods and capabilities could increase international confidence in findings.

Considerations

- Federal agencies often have different goals and requirements, so even with increased coordination, efficiencies may be limited.

[27]GAO, *National Biodefense Strategy: Additional Efforts Would Enhance Likelihood of Effective Implementation*, GAO-20-273 (Washington, D.C.: Feb. 19, 2020)

[28]OPCW has performed similar exercises in related fields such as toxin identification.

- Confidence-building exercises are typically voluntary, and without additional support they could divert resources from other tasks.
- Confidence-building exercises in this area would require classification and sensitivity issues to be worked out in advance.

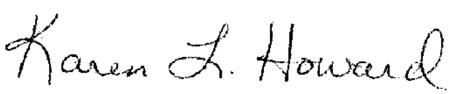
5 Agency and Expert Comments

We provided a draft of this product to the Department of State, Department of Health and Human Services, Department of Defense, Department of Commerce, Department of Energy, Department of Justice, Department of Homeland Security, and the Office of the Director of National Intelligence with a request for technical comments. Six agencies provided us with technical comments, which we incorporated as appropriate.

We invited the participants from our meeting of experts to review our draft report. Of the experts, seven reviewed our draft report, and we incorporated comments as appropriate.

We are sending copies of this report to the appropriate congressional committees and interested parties. In addition, the report is available at no charge on the GAO website at https://www.gao.gov.

If you or your staff have any questions about this report, please contact me at 202-512-6888 or howardk@gao.gov. Contact points for our Offices of Congressional Relations and Public Affairs may be found on the last page of this report. GAO staff who made contributions to this report are listed in Appendix IV.



Karen L. Howard, PhD
Acting Chief Scientist and Director
Science, Technology Assessment, and
Analytics (STAA)

List of Addressees

The Honorable Ted Cruz
Ranking Member
Committee on Commerce, Science, and Transportation
United States Senate

The Honorable Gary C. Peters
Chairman
The Honorable Rand Paul, M.D.
Ranking Member
Committee on Homeland Security and Governmental Affairs
United States Senate

The Honorable Mark Warner
Chairman
The Honorable Marco Rubio
Vice Chairman
Select Committee on Intelligence
United States Senate

The Honorable Mike Rogers
Chairman
The Honorable Adam Smith
Ranking Member
Committee on Armed Services
House of Representatives

The Honorable Frank Lucas
Chair
The Honorable Zoe Lofgren
Ranking Member
Committee on Science, Space, and Technology
House of Representatives

Appendix I: Objectives, Scope, and Methodology

Objectives

This report discusses:

1. The status of key technologies available to identify a chemical agent and its source, including their strengths and limitations;
2. Challenges researchers and investigators face in trying to identify a chemical agent or its source; and
3. Policy options that may help address the challenges of using key technologies to identify a chemical agent and its source.

Scope and methodology

To address our three objectives, we assessed available and developing technologies that are currently used to identify a chemical agent and its source. For all of our objectives we reviewed key reports, peer-reviewed scientific literature, and other documents describing current and developing technologies, including reports from the Organisation for the Prohibition of Chemical Weapons (OPCW), and select national laboratories; interviewed representatives from the OPCW, and federal agencies and laboratories, as well as experts from academia, OPCW-certified laboratories, and non-profit organizations; and convened two expert meetings with assistance from the National Academies of Sciences, Engineering, and Medicine to discuss the objective topics.

Limitations to scope

The list of key technologies to identify a chemical agent and its sources discussed in this report is not intended to be exhaustive. Based on our review of the literature and discussion with federal agency officials and other experts, we selected technologies currently in use or in development by researchers to identify chemical agents and their sources. Since identifying a chemical agent and its source may require international efforts, the policy options we identified represent possible actions U.S. policymakers and international stakeholders could take.

Literature search

In the course of our review, we worked with a GAO research librarian to conduct a literature search of key technologies for identifying a chemical agent and its source. The librarian conducted literature searches with Scopus using search terms including “attribution”, “technology”, “chemical weapons”, and “impurity profiling”, among other keywords relevant to technologies for identifying a chemical agent and its source. We conducted a broad search of materials published within the last 10 years, including scholarly articles and government reports. From these searches, we identified and selected relevant articles to include in our review. We used the results of our literature review to inform our findings as well as identify experts to interview or invite to participate in our expert meeting.

Interviews

We interviewed federal agency officials and researchers as well as nonfederal experts with a diverse set of perspectives on the science and application of these technologies. These experts included individuals from relevant federal agencies: the Department of State, Department of Defense, Department of Homeland Security, Department of Energy, Department of Health and Human Services' Centers for Disease Control and Prevention, Department of Justice's Federal Bureau of Investigation, and National Institute of Standards and Technology. We also interviewed experts from the OPCW and a select portion of its designated laboratories. We also interviewed experts from domestic and international universities involved in identifying a chemical agent or its source. In addition, we attended a chemical forensic symposium at the Fall 2022 American Chemical Society conference.

Expert meeting

To address all of our objectives, we also held two expert meetings on May 19-20, 2022, and June 22, 2022. These meetings were held with assistance from the National Academies of Sciences, Engineering, and Medicine (National Academies). However, all final decisions regarding meeting substance and expert participation are the responsibility of and were made by GAO. We selected meeting participants based on their expertise in at least one area related to our three objectives. We provided the National Academies with descriptions of the expertise needed by expert meeting participants. From this information, the National Academies provided an initial list of potential participants for the expert meetings. We reviewed the list and provided an additional list of experts.

In addition to evaluating experts on the basis of their expertise, we evaluated them for any conflicts of interest. A conflict of interest was considered to be any current financial or other interest, such as an organizational position, that might conflict with the service of an individual because it could (1) impair objectivity or (2) create an unfair competitive advantage for any person or organization. Of the 23 experts who participated in the expert meetings, some were affiliated with companies, government, or research-funding entities. We took these affiliations into consideration as potential conflicts of interest when conducting our analysis and preparing our report. We determined that these experts' affiliations were unlikely to bias our overall reporting.

Site visits

To learn about the various chemical forensic approaches and technologies that exist or are being developed, as well as interview subject matter experts about their expertise, we visited the Army Combat Capabilities Development Command Chemical Biological Center, the National Nuclear Security Administration's Lawrence Livermore National Laboratory, and the Department of Energy's Pacific Northwest National Laboratory.

Policy options

Based on our research, we developed a series of policy options. Policy options are intended to represent possible options policymakers can take to address a policy objective. For each policy option, we discussed potential opportunities and considerations. These are not listed in any particular order, nor are they inclusive of all possible policy options. Based on the goal of improving abilities to identify a chemical agent and its source, we decided on an objective designed to identify options that could help improve these abilities. We limited policy options to those that fit the objective and fell within the report scope.

To develop our policy options, we compiled a list of possible options over the course of our work based on review of the literature, interviews with experts, and our expert meetings held May 19-20, 2022, and June 22, 2022. We further refined and assessed these options to ensure they were adequately supported by the evidence we collected, could be feasibly implemented, and fit into the overall scope of our work. We then analyzed the information we collected to identify potential benefits and considerations of implementing each policy option. The policy options and analyses were supported by documentary and testimonial evidence.

We conducted our work from September 2021 to September 2023 in accordance with all sections of GAO’s Quality Assurance Framework that are relevant to technology assessments. The framework requires that we plan and perform the engagement to obtain sufficient and appropriate evidence to meet our stated objectives and to discuss any limitations to our work. We believe that the information and data obtained, and the analysis conducted, provide a reasonable basis for any findings and conclusions in this product.

Appendix II: Expert Participation

With the assistance of the National Academies of Sciences, Engineering, and Medicine we convened two meetings of experts to inform our work on current and emerging technologies for chemical weapon forensic attribution. The first expert meeting was held on May 19-20, 2022, and the second was held on June 22, 2022. The experts who participated in the meetings are listed below. The experts gave us additional assistance throughout our work, including providing additional technical assistance during our study by sending additional technical material for our review, or answering technical questions; and seven experts reviewed our draft report for accuracy and provided technical comments.

First expert meeting—Participants

Marc-Michael Blum

Independent Consultant

Blum-Scientific Services

Carlos Fraga

Chief

Propellants Branch, Air Force Research Laboratory

Cesar Metzger

Head

Chemical, Biological, Radiological, and Nuclear Coordination Unit, Spiez Laboratory

Andy Nong

Acting Manager

Exposure and Biomonitoring Division, Health Canada Environmental Health Sciences and Research Bureau

Robert Synovec

Professor

Department of Chemistry, University of Washington

Paula Vanninen

Director

Finnish Institute for Verification of the Chemical Weapons Convention, Department of Chemistry, University of Helsinki

Second expert meeting—Participants[29]

Armando Alcaraz

Project Leader

Forensic Science Center, Lawrence Livermore National Laboratory

Douglas Anders

Senior Scientist

Chemical, Biological, Radiological, and Nuclear and Forensic Response, Federal Bureau of Investigation (FBI)

[29] An additional official from the Federal Bureau of Investigation attended the second expert meeting. The official's name is withheld per the agency's request.

John Cort

Chemist

Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory

David C. Dorman

Professor

Toxicology, North Carolina State University

Jonathan Forman

Science and Technology Advisor

National Security Directorate, Pacific Northwest National Laboratory

Gary S. Groenewold

Senior Scientist (Retired)

Idaho National Laboratory

Robert Kristovich

Chief

Threat Agent Sciences Division, U.S. Army

Gary Mallard

Sole Proprietor

Teal Consulting

Kathleen McCormac-Miller

Physical Scientist

U.S. Department of State

Randall Murch

Associate Director

Research Program Development, National Capital Region, Virginia Tech

Janelle Newman

Principal Chemist

MRIGlobal

Sara Peacock

Senior Science and Technology Manager

Defense Threat Reduction Agency

Sherrie Pilkington

Program Manager

Intelligence Advanced Research Projects Activity

David Reif

Professor

Toxicology, North Carolina State University

Kabrena Rodda

Group Lead

National Security Directorate, Pacific Northwest National Laboratory

Paul Walker

Vice Chair

Board of Directors, Arms Control Association

Appendix III: Selected Analytical Instrumentation

Table 4: Selected Analytical Instrumentation

Technology	What it does	Strengths	Limitations
Gas chromatography (GC)	Separates individual chemicals in a sample mixture by vaporizing and passing through a column.	Relatively simple to use. Commonly used in a variety of industries. Can work with micrograms (millionths of a gram) of sample.	Limited to samples that can be converted into the gaseous phase for analysis.
Liquid chromatography (LC)	Separates individual chemicals in a sample mixture by dissolving in solvent and passing through a column.	Capable of identifying a broad range of chemicals, including those that do not vaporize easily or those that are heat-sensitive. Can work with micrograms of sample.	More complex than GC. Limited reference data.
Mass spectrometry (MS)	Provides information about a chemical's formula and identity based on the mass-to-charge ratio of their ions.	High selectivity, high sensitivity, and the availability of reference databases. Versions of MS are compatible with both GC and LC. Specialized MS instruments can measure isotope ratios. Can work with micrograms of sample.	Can be complex to use. Limited resolution and limits of detection can sometimes hinder the ability to analyze complex samples. The technique is destructive; samples inserted into instruments are destroyed and cannot be reused.
Gas chromatography-mass spectrometry (GC-MS)	Combines GC and MS for improved detection. Data generated by this method can be analyzed to provide high confidence chemical identification.	Highly sensitive method that can detect compounds in extremely diluted samples, often at the parts per billion level. Can work with a few microliters of sample. Reference data for thousands of compounds are available for comparison.	Samples containing chemicals that are difficult to separate by GC and give similar signals in MS can lead to identification errors. The technique is destructive; samples inserted into instruments are destroyed and cannot be reused.

Technology	What it does	Strengths	Limitations
High-resolution mass spectrometry (HRMS)	Provides precise mass-to-charge ratios with a resolution at least 20 times higher than that of conventional MS systems. This provides an increased ability to identify chemicals in a complex sample.	Enhanced resolution makes it possible to distinguish various isotopes of atoms and significantly reduces chemical interferences during analysis of complex samples, thereby improving the accuracy of chemical formula prediction and library matching for compound identification. HRMS may provide precise enough information about chemicals in a sample that reference data may no longer be needed, which could reduce reliance on databases.	Equipment is expensive and generates large quantities of complex data which may not be necessary for routine analyses of compounds. Requires trained personnel with expertise in data interpretation. The technique is destructive; samples inserted into instruments are destroyed and cannot be reused.
Infrared spectroscopy (IR)	Provides information about the chemical structure of a molecule, such as how various atoms are grouped within the molecule. This can be used to identify parts of a molecule and differentiate between closely related compounds.	Fast and non-destructive analysis used in the detection of a wide variety of chemicals. Available in hand-held, fieldable instruments	Requires milligrams (thousandths of a gram) of sample, which is much more than some other methods. May not be suitable for analysis of mixtures. Challenging to use with samples in water. Usefulness may be limited when no reference data are available.
Raman spectroscopy	Provides information about the chemical structure of a molecule, such as how various atoms are grouped within the molecule. This can be used to identify parts of a molecule and differentiate between closely related compounds.	Fast and non-destructive analysis. Does not require contact with samples. Handheld Raman instruments are commercially available.	Requires milligrams of sample. Not suitable for analysis of mixtures. Usefulness may be limited when no reference data are available.

Technology	What it does	Strengths	Limitations
Nuclear magnetic resonance (NMR) Spectroscopy	Provides information about how specific groups of atoms within a chemical are connected. Works with hydrogen, carbon, fluorine, and phosphorus atoms, which are present in many chemical agents.	Can be used to determine molecular structure of unknown chemicals or conduct isotope ratio measurements. Portable instruments can be taken into field. Can provide quantitative results and is non-destructive.	Requires milligrams of sample. The most sensitive NMR instruments have significant infrastructure requirements and need trained personnel with technical expertise for operation. Usefulness may be limited when no reference data are available.

Source: GAO analysis of government, commercial documents and interviews with experts. | GAO-23-105439

Appendix IV: GAO Contact and Staff Acknowledgments

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