

### **Scientific Advisory Board**

SAB-40/WP.2 27 August 2025 ENGLISH only

### SUMMARY OF THE FIFTH MEETING OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP ON CHEMICAL FORENSICS

- 1. AGENDA ITEM ONE Opening of the meeting and adoption of the agenda
- 1.1 The Temporary Working Group (TWG) on Chemical Forensics of the Scientific Advisory Board (SAB) held its fifth meeting from 11 to 13 June 2025 at the Finnish Institute for Verification of the Chemical Weapons Convention (VERIFIN) in Helsinki, Finland. The meeting was chaired by Dr Anne Bossée on behalf of the SAB, with Dr Simon Ovenden as Vice-Chairperson.
- 1.2 Dr Bossée opened the fifth meeting of the TWG by welcoming its members and the external speakers. She acknowledged the valuable contributions that the presentations of the expert speakers bring to the findings of the Group. She noted that virtual meetings of the subgroups had taken place during the intersessional period. The Chairperson and Vice-Chairperson then updated the TWG on the status of the draft end-of-mandate report, describing the approach that had been adopted so far. They encouraged the TWG members to review the current draft text and provide comments and additional input as required. Finally, Dr Bossée invited all participants to introduce themselves; a list of participants appears in the Annex to this report.
- 1.3 As no objections or comments were raised in response to the proposed programme of work during the three days of the meeting, the following agenda was adopted:
  - 1. Opening of the meeting and adoption of the agenda
  - 2. Updates from subgroups<sup>1</sup>
  - 3. Breakout session Subgroups 1 and 4<sup>2</sup>
  - 4. Breakout session Subgroups 2 and 3<sup>3</sup>
  - 5. Position-specific isotope analysis utilising nuclear magnetic resonance spectroscopy
  - 6. Tracking chemical casualties in conflict zones challenges and forensic analytical trends



While agenda items 2, 3, 4, 11, and 12 were discussed separately during the meeting, they are reported herein under a single agenda item for clarity and to minimise duplication.

<sup>&</sup>lt;sup>2</sup> Ibid.

<sup>3</sup> Ibid.

- 7. Forensic chemistry findings: probabilistic evaluation and data requirements
- 8. Nuclear forensics how databases are used in interpreting results
- 9. Icarus: chemical forensics sample matching exercise 2025
- 10. Privacy-enhancing technologies in data and AI systems
- 11. Breakout sessions Subgroups 1 and 2 (together) and Subgroups 3 and 4 (together)<sup>4</sup>
- 12. Group discussion<sup>5</sup>
- 13. Closing remarks and any other business
- 14. Closure of the meeting

## 2. AGENDA ITEMS TWO, THREE, FOUR, ELEVEN, AND TWELVE – Discussion on subgroup topics

- 2.1 Subgroup 1, led by Dr Crister Åstot, is focusing on the state of the art of chemical forensics, and is considering the areas of batch matching, impurity profiling, synthesis routes, geographical and environmental factors, and isotope ratios. In discussions during previous meetings, Subgroup 1 had noted the lack of ground truth reference data relating to chemical warfare agents. The need for reference data was discussed at length during this fifth TWG meeting, particularly in relation to the development of a chemical forensics database. The subgroup also discussed how States Parties could be encouraged to share their data in this regard.
- 2.2 Several presentations during the fifth TWG meeting were particularly relevant to the work of Subgroup 1 and inspired further discussion. For example, Dr Cornelia Rasmussen has developed a technique using nuclear magnetic resonance (NMR) spectroscopy that detects absolute ratios of carbon-13 to carbon-12 (\(^{13}\text{C}/^{12}\text{C}\)) at individual carbon sites (see agenda item 5). While carbon-13 satellite peaks in proton NMR have previously been leveraged for isotopic fingerprinting of chemicals, the position-specific isotope analysis technique developed by Dr Rasmussen and her team is a promising alternative and can provide additional insights on the origin of a molecule.
- 2.3 Subgroup 1 also further considered the presentation given by Dr Anders Nordgaard on the probabilistic assessment of forensic findings (see agenda item 7). This presentation complemented previous discussions of the subgroup on applying likelihood ratio-based statistical tools to support expert opinions in investigations, including those involving chemical weapons. The subgroup discussed the reference-data requirements for the application of the statistical methods presented by Dr Nordgaard in the field of forensic statistics. It was agreed that explanatory text on such a probabilistic statistical approach would be included in the end-of-mandate report.

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<sup>4</sup> Ibid.

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- 2.4 Subgroup 2, led by Dr Grégoire Delaporte, is addressing future capabilities, focusing on the impact of artificial intelligence (AI), specifically machine learning (ML) and deep learning, on chemical forensics. During the intersessional period, the subgroup continued discussing and refining its draft recommendations for the end-of-mandate report. While the subgroup has proposed several recommendations in response to questions 7(a) and 7(b) of the terms of reference of the TWG, it agreed that additional input would be required to formulate recommendations with respect to question 7(c). Subgroup 2 proposed that it would be beneficial to engage with key expert speakers who had presented at previous meetings of the TWG, and suggested that a questionnaire would be the most appropriate means of facilitating this discussion. The questionnaire will include three questions regarding obstacles, possibilities, and potential technological game changers in the respective fields of the experts identified.
- Ms Ang Lee Hwi, Subgroup 3 lead, provided an update on progress in reviewing international standards and guidelines for forensic science. She noted that a comparison has been made between International Organization for Standardization/International Electrotechnical Commission (ISO/IEC) standards 17025 and ISO/IEC 17020—which currently form the backbone of forensic science accreditation—and the newly published ISO 21043 standard for forensic science. The subgroup has identified specific requirements relevant to forensic science that would supplement ISO/IEC 17025 and ISO/IEC 17020, for recommendation in the end-of-mandate report. For analysis, these include requirements in measurement uncertainty, performance monitoring, acceptance and rejection of requests and items, analytical strategy, purpose of analysis, and reliability of observations. For on-site sampling, there are requirements relating to health and safety, initial response at scenes, forensic examinations, and item handling and control. Standard ISO 21043 also provides the specific requirements for interpretation and reporting.
- 2.6 Subgroup 3 proposed possible approaches to combining data from different techniques, including the generation of leads from different techniques, followed by expert interpretation, and the use of multi-block algorithms in chemometrics. A possible approach to preserving data privacy through a local differential privacy model was also shared with the wider TWG.
- 2.7 During the breakout sessions, Subgroup 3 further discussed the review of international standards and guidelines for forensic science. The subgroup underscored the importance of maintaining a quality management system in accordance with ISO/IEC 17025 and ISO/IEC 17020 in laboratories conducting forensic analysis and sampling of chemical warfare agents and related substances. Subgroup 3 also noted that the Technical Secretariat (the Secretariat)—and possibly the Forensic Adviser in particular—could play an important role in assessing the suitability of the laboratories to follow the specific requirements. It was highlighted that the Secretariat may undertake interpretation and reporting in consultation with the laboratories conducting forensic analyses. Consequently, the requirement for interpretation and reporting should apply to the Secretariat instead of the laboratories. Subgroup 3 proposed that, to facilitate this role, the Forensic Adviser should be familiar with ISO 21043.

The complete terms of reference of the TWG on Chemical Forensics are provided in Annex 1 to SAB-38/WP.1 (dated 15 May 2024).

- 2.8 The subgroup also discussed combining data from different techniques, and concerns were raised about the robustness of the multi-block algorithm used in chemometrics for this purpose. Subgroup 3 will review relevant references on this topic and discuss with Subgroup 2 to assess the suitability of the approach. It was agreed that, regardless of the approach, expert assessment remains an important final step.
- 2.9 The common breakout session between Subgroups 2 and 3 focused initially on the proposed chemical forensics database. The discussions highlighted the need for a large-scale chemical forensics database that is machine-readable so that it may be effectively used by AI/ML methods. Subgroups 2 and 3 also discussed the possible redesign of the environmental proficiency test to ensure that it is testing proficiency in the most relevant needs of the OPCW, increasingly related to authentic samples from non-routine missions. It was proposed that the proficiency test scenario should incorporate chemical forensics questions. The scope of analysis for the proficiency test could remain as the verification of Chemical Weapons Convention-related chemicals, while additional questions on forensics (such as sample matching, chemical warfare agent-precursor attribution, and/or route tracing) may be posed in an optional exercise that may include additional samples if necessary.
- 2.10 The discussions of Subgroup 4, led by Dr Hanna Hakulinen, centred primarily on the development of the proposed database and the chemical forensics workflow. The subgroup proposed a two-part structure for the database.
- 2.11 The first part would be the knowledge hub, which would contain existing literature and reference data, and be designed to be queried once specific forensic questions have been defined. This would serve as a repository of established information to support investigative efforts. Subgroup 4 members noted that the effective use of this knowledge hub would require clearly defined forensic questions, standardised terminology, and a well-scoped analytical framework. They suggested that typical forensic questions may include sample or batch matching, route sourcing, precursor-product relationships, dissemination pathways, and storage and degradation patterns. It was emphasised throughout the discussion that all investigative events begin as verification events. Once the forensic questions are defined, the knowledge hub can be queried to retrieve relevant information that guides subsequent investigations.
- 2.12 The second part—a database—would contain route-specific data, including impurity profiles and other analytical markers. It would be modelled on the format of the Validation Group Working Database (VGWD) and would aim to support detailed forensic comparisons.
- 2.13 To ensure usability, the entire database should have a clear and straightforward entry point that can be expanded over time. The subgroup agreed that immediate action is required with respect to this database creation, and that realistic, actionable recommendations from the TWG are essential for progress.
- 2.14 During these discussions, Subgroup 4 identified a number of key challenges. These included data-sharing protocols, criteria for forensic data inclusion, and accuracy and consistency (for example, typographical errors in submitted data). Despite these challenges, it was agreed that the proposed approach offers significant advantages, particularly in fostering collaboration between laboratories.

- 2.15 In addition to proposing a database structure, Subgroup 4 also proposed a chemical forensics workflow, which is designed to be general and adaptable across various forensic scenarios. The steps proposed were to:
  - (a) define the forensic questions;
  - (b) conduct necessary analyses;
  - (c) analyse data and consult existing databases (such as the OPCW Central Analytical Database and the VGWD) and AI-based tools;
  - (d) query the knowledge hub;
  - (e) generate a "hit list" of relevant markers and perform qualitative assessments; and
  - (f) use the chemical forensics peak list to produce outputs that may lead to likelihood ratios or other forensic conclusions.
- 2.16 Subgroup 4 agreed that successful implementation of the workflow would require multidisciplinary expertise, including in synthetic chemistry, analytical chemistry, and chemometrics and statistics. Furthermore, external laboratories could be engaged, as required, to support specific aspects of the workflow. Lastly, Subgroup 4 noted that the sampling questions that are being discussed in Subgroup 3 are also particularly relevant in this context.
- 3. AGENDA ITEM THREE Breakout session Subgroups 1 and 4

See agenda item 2.

4. AGENDA ITEM FOUR – Breakout session – Subgroups 2 and 3

See agenda item 2.

- 5. AGENDA ITEM FIVE Position-specific isotope analysis utilising nuclear magnetic resonance spectroscopy
- 5.1 Dr Cornelia Rasmussen from the University of Texas at Austin, United States of America, presented an overview of the application of NMR spectroscopy in advancing forensic identification, focusing on a novel approach to position-specific carbon isotope analysis. Unlike isotope ratio mass spectrometry methods that produce a global isotope composition, Dr Rasmussen and her team have developed a technique using NMR spectroscopy that detects absolute ratios of <sup>13</sup>C/<sup>12</sup>C at individual carbon sites. This is achieved via indirect detection through superposition of satellite peaks using various nuclei, such as hydrogen, phosphorus, and fluorine. Their innovative approach, improving the sensitivity and selectivity of the technique, has been successfully applied to a wide range of substances, such as pharmaceuticals, pesticides, amino acids, and nucleosides.
- 5.2 The findings demonstrate that each molecule retains a distinct intramolecular carbon isotope fingerprint, influenced by its biosynthetic or chemical formation pathway. This technique has the potential to identify the source of a compound, its method of synthesis, and link degradation products back to their original substances. As a result, the technique enhances forensic capabilities for tracing the origin and transformation of chemical compounds. Beyond chemical forensics, the implications extend to environmental science, geochemistry, and even astrobiology, where tracing molecular origin and transformation is of growing importance.

5.3 After the presentation, TWG members raised technical questions about the accuracy and limitations of peak integration for carbon ratios, challenges with long signal tails, and the use of principal component analysis to detect outliers and reduce noise in large datasets. Additional questions addressed the time and complexity of data analysis, required skill sets, automation potential, and the resolution of overlapping signals in mixtures using a 600 MHz NMR instrument, particularly in complex or modified biological systems.

# 6. AGENDA ITEM SIX – Tracking chemical casualties in conflict zones – challenges and forensic analytical trends

- 6.1 Prof. Sermet Sezigen, from the University of Health Sciences, Türkiye, gave an overview of various aspects of tracking chemical casualties. He presented the challenges faced in conflict zones, emerging forensic analytical trends, and the importance of collecting biomedical samples from sulfur mustard casualties.<sup>7</sup>
- Prof. Sezigen underlined the importance of collecting biomedical samples, such as blood, urine, hair, and tissues. Such samples are vital not only for verifying the use of chemical weapons but also for supporting criminal investigations and informing medical and humanitarian responses. However, he emphasised that collecting these samples in conflict zones presents significant technical, logistical, and political challenges, which can affect the reliability and legal validity of the forensic evidence. Prof. Sezigen outlined several of these obstacles, including the lack of infrastructure, high ambient temperatures, absence of cold-chain logistics, and shortages of sampling kits and personal protective equipment. These issues often lead to compromised sample integrity and preservation. To overcome the current challenges, he suggested establishing mobile forensic response units. These would be trained in handling chemical agent exposure cases, prioritising matrices with longer detection windows, and training local health workers in basic forensic sampling. He further emphasised that addressing these challenges requires both coordinated international efforts and a multilateral, multidisciplinary, strategic, and culturally sensitive approach.
- 6.3 In terms of analytical trends, Prof. Sezigen advocated for the use of stable and easily collected matrices such as hair, dried blood, or plasma. These sample types are suitable for field collection without refrigeration and compatible with advanced analytical techniques, making them highly effective for verifying exposure to chemical agents. Additionally, they enable robust, reliable, and practical sampling and analysis, especially when conventional refrigerated storage and transport are unfeasible.
- 6.4 The subsequent discussion focused on challenges in post-mortem toxicology, the chain of custody, and technical constraints of current equipment. TWG members suggested that designated laboratories could be encouraged to analyse hair and dried blood samples during the biomedical proficiency tests to confirm nerve agent or sulfur mustard exposure. With the increasing sensitivity of analytical techniques, TWG members encouraged conducting metabolism studies for different chemical warfare agents from several production routes. This would enable the evaluation of the possibility of using biomedical sample analysis as part of a forensic investigation.

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John, Harald, Sophia Willoh, Philipp Hörmann, Markus Siegert, Antje Vondran, and Horst Thiermann. "Procedures for Analysis of Dried Plasma Using Microsampling Devices to Detect Sulfur Mustard-Albumin Adducts for Verification of Poisoning." *Analytical Chemistry* 88, no. 17 (August 15, 2016): 8787–94. https://doi.org/10.1021/acs.analchem.6b02199.

# 7. AGENDA ITEM SEVEN – Forensic chemistry findings: probabilistic evaluation and data requirements

- 7.1 Dr Anders Nordgaard from the National Forensic Centre of the Swedish Police Authority presented on the probabilistic assessment of forensic findings. He outlined how probability calculations and statistical methods aid in decision-making about judicial statements, such as "the chemical weapon used in attack A has the same origin as the one used in attack B."
- 7.2 Dr Nordgaard commenced his presentation by discussing how evidentiary strengths can be evaluated through probabilistic mathematical calculations. Broadly, the calculations determine how likely a prior judicial statement—such as that two separate cocaine seizures come from the same batch—is to be true, given certain chemical forensic evidence (for example, the concentration of cutting agents in a cocaine seizure). The probabilistic calculations aim to identify the odds of a statement being true or false given chemical forensic evidence, while also accounting for prior beliefs held about the statement by the legal factfinder. The strength of support for a statement is mathematically expressed by the likelihood ratio, which is crucial for answering forensic questions.
- 7.3 In contrast to chemical questions—such as identifying a substance or determining its concentration within a sample—forensic questions often carry a greater degree of uncertainty. Examples include determining whether fire debris contains traces of ignitable liquids, or whether hazardous waste was burnt at the site of a fire. This increased uncertainty requires forensic questions to be communicated through probability and likelihood ratios. To deduce likelihood ratios, chemometrics—the science of using statistical-mathematical methods to extract information from chemical data—can be a useful approach. If the forensic question concerns the class to which a seized sample belongs (for example, determining whether seized amphetamine was produced in the Netherlands, Finland, or Sweden), discriminant analysis can be applied to calculate likelihood ratios.
- 7.4 When the forensic question pertains to the origin of a sample or whether two samples share a common origin, other probabilistic models and methods of chemometrics need to be applied to calculate likelihood ratios. In this case, the forensic question can be evaluated by using either a feature- or score-based approach. Comparing both approaches, Dr Nordgaard noted that the score-based approach is less powerful than the feature-based one. However, it is easier to apply to datasets with a large number of variables like chemical profiles. It was additionally emphasised that sufficient reference data is needed to ensure the reliability of score-based evaluation. 9

Ahrens, Björn, Ivo Alberink, Michael Bovens, Sami Huhtala, Anders Nordgaard, and Tuomas Salonen. *Guideline for the use of chemometrics in forensic chemistry*. Wiesbaden: European Network of Forensic Science Institutes, 2020.

Leegwater, Anna Jeannette, Peter Vergeer, Ivo Alberink, Leen V. van der Ham, Judith van de Wetering, Rachid El Harchaoui, Wauter Bosma, Rolf J.F. Ypma, and Marjan J. Sjerps. "From Data to a Validated Score-Based LR System: A Practitioner's Guide." *Forensic Science International* 357 (April 2024): 111994. https://doi.org/10.1016/j.forsciint.2024.111994.

7.5 Following the presentation, questions were raised regarding the score-based approach, the minimum number of reference samples required, and the establishment of a score-based model for chemical agents through laboratory collaboration.

# 8. AGENDA ITEM EIGHT – Nuclear forensics – how databases are used in interpreting results

- 8.1 Dr Maria Wallenius, from the Nuclear Safety and Security Unit of the European Commission's Joint Research Centre (JRC), outlined the critical role nuclear forensics plays in ensuring nuclear security, with particular emphasis on the indispensable contribution of databases to nuclear forensic analysis.
- 8.2 Dr Wallenius explained that in cases where nuclear material is discovered outside of regulatory control, nuclear forensics aims to determine the composition of the material, its origin, method and date of production, intended use, and potential links to other cases. To answer these questions, nuclear forensic signatures (characteristic sample parameters) are studied, allowing one sample to be distinguished from another. Signatures such as stable isotope ratios or impurities from rare earth elements can be related to the geological origin of a sample. Other signatures, such as morphology, surface roughness, or age, may be associated with the post-mining processing of the material. Additionally, forensic signatures can be grouped into two categories: predictive (no comparative data needed) and comparative (reference data required).
- 8.3 To answer questions related to unknown nuclear materials, Dr Wallenius emphasised the importance of databases in nuclear forensics, allowing for systematic comparison of a sample with reference data. In the mid-1990s, the JRC began compiling data on nuclear fuel pellets, stemming from open sources, fuel manufacturers, specific data cases, and research results from studies performed at the Centre. The database is classified into core data (including pellet dimensions and main elements), extended data (such as roughness), and complementary data (for example, electron microscopy images). Security and confidentiality are paramount in managing the database. Confidentiality agreements were signed with fuel pellet manufacturers to protect sensitive data, and only authorised JRC personnel are allowed to query the database following a request from a country conducting nuclear forensic analysis. Dr Wallenius presented a specific example in which the database was indispensable in tracking down the source of uranium pellets found in Germany.
- 8.4 Dr Wallenius concluded her presentation by providing an overview of the Nuclear Forensics International Technical Working Group (ITWG). As an informal association of official practitioners of nuclear forensics (scientists, law enforcement officers, first responders, and nuclear regulators), the ITWG focuses on advancing the nuclear forensics scientific discipline, fostering collaboration, providing a common approach, and developing technical solutions.
- 8.5 Task groups are an essential part of the activities of the ITWG. The Exercises Task Group facilitates laboratory-based exercises on nuclear material, providing learning opportunities for participants. The Libraries and Assessment Task Group directly contributes to database development by providing guidance on the implementation of national nuclear forensics libraries (NNFLs). These libraries can assist countries in determining whether nuclear material found outside of regulatory control had been

produced, used, or stored within their borders. To increase national capabilities regarding the NNFLs, the "Galaxy Serpent" virtual training exercise is conducted regularly.

8.6 The TWG members noted striking commonalities—particularly in approaches and challenges—between the fields of nuclear and chemical forensics related to chemical warfare agents and raised several questions in this regard. They were particularly interested in the JRC nuclear materials database, the NNFLs, and frequency of updates; access to and security of the nuclear materials database; understanding how confidentiality is addressed; the application of AI tools; and data validation.

### 9. AGENDA ITEM NINE – Icarus: chemical forensics sample matching exercise 2025

- 9.1 Dr Carlos Fraga, from the United States Air Force Research Laboratory, opened his presentation with an overview of the background that led to the development of the Icarus exercise, a chemical forensics sample matching exercise taking place in 2025. He then provided a detailed description of the exercise itself, including the requirements, participants, and the schedule, from sample shipping to results reporting.
- 9.2 The United States Department of Homeland Security Chemical Forensics Program was active between 2006 and 2017 and involved multiple domestic laboratories as well as the Swedish Defence Research Agency (FOI). The scientific papers produced during this period laid the foundation for the chemical forensics attribution of chemical threat agents. Methylphosphonic dichloride (DC), a commercially available precursor of G-series nerve agents, was used as a model compound in the Chemical Forensics Program, where its impurities were extensively analysed using gas chromatography-mass spectrometry (GC-MS), NMR spectroscopy, liquid chromatography-mass spectrometry (LC-MS), and isotope ratio mass spectrometry. <sup>10,11,12</sup>
- 9.3 Dr Fraga introduced the Chemical Forensics International Technical Working Group (CFITWG), which held its inaugural meeting in 2017. This working group was established to address gaps in chemical forensics science and capabilities through international partnerships of experts from scientific, policy, academic, law enforcement, and export-control organisations. Dr Fraga provided an overview of the

Fraga, Carlos G., Gabriel A. Pérez Acosta, Michael D. Crenshaw, Krys Wallace, Gary M. Mong, and Heather A. Colburn. "Impurity Profiling to Match a Nerve Agent to Its Precursor Source for Chemical Forensics Applications." *Analytical Chemistry* 83, no. 24 (November 22, 2011): 9564–72. <a href="https://doi.org/10.1021/ac202340u">https://doi.org/10.1021/ac202340u</a>.

Fraga, Carlos G., Brian H. Clowers, Ronald J. Moore, and Erika M. Zink. "Signature-Discovery Approach for Sample Matching of a Nerve-Agent Precursor Using Liquid Chromatography–Mass Spectrometry, XCMS, and Chemometrics." *Analytical Chemistry* 82, no. 10 (April 21, 2010): 4165–73. <a href="https://doi.org/10.1021/ac1003568">https://doi.org/10.1021/ac1003568</a>.

Moran, James J., Carlos G. Fraga, and Megan K. Nims. "Stable-Carbon Isotope Ratios for Sourcing the Nerve-Agent Precursor Methylphosphonic Dichloride and Its Products." *Talanta* 186 (August 15, 2018): 678–83. https://doi.org/10.1016/j.talanta.2018.04.021.

CFITWG projects.<sup>13,14</sup> He then focused on the "DC project" in more detail and highlighted two scientific articles showcasing the project results.<sup>15,16</sup> Finally, Dr Fraga underscored the importance of the latest edition of the Blue Book, which contains recommended operating procedures for chemical attribution techniques (such as sample matching, route attribution, and position-specific isotope analysis), quality control, and chemometrics.<sup>17</sup>

- 9.4 The Icarus exercise was created to meet several needs, including testing techniques that had been demonstrated separately in proof-of-concept papers and extending and improving chemical profiling and sample matching. Icarus has been designed to assess the current state of the art and identify areas for further study and improvement in chemical profiling. Dr Fraga noted that Icarus will use "wet" (laboratory-based) sample matching to determine whether samples of chemical warfare agent simulants could be matched to other samples from the same source and to their precursors from specific sources. He outlined the various requirements for the participating laboratories, highlighting the analytical techniques that will be employed. In closing, Dr Fraga explained the differences between Tier 1 and Tier 2 forensic questions and corresponding samples.
- 9.5 In the discussion that ensued, the TWG members agreed that the Icarus exercise will provide results that will play an important role in developing the field of chemical profiling. They noted that the exercise will be useful in revealing the analytical variation across a large number of samples, not only for GC-MS analysis, but also for other key techniques. Dr Fraga noted that areas such as standardisation and analytical techniques other than GC-MS will still require further attention and development in the future. Next steps will include developing a suitable quality control test mixture for LC-MS and producing additional chapters for the next edition of the Blue Book, among others. The Group also discussed potential avenues for generating more analytical data to bolster the capability further and the anonymisation of data to enhance privacy and security.

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Ovenden, Simon P. B., Renée L. Webster, Eva Micich, Lyndal J. McDowall, Nathan W. McGill, Jilliarne Williams, and Shannon D. Zanatta. "The Identification of Chemical Attribution Signatures of Stored VX Nerve Agents Using NMR, GC-MS, and LC-HRMS." *Talanta* 211 (May 1, 2020): 120753. https://doi.org/10.1016/j.talanta.2020.120753.

Hemme, Maria, Alex Fidder, Debora van der Riet-van Oeveren, Marcel J. van der Schans, and Daan Noort. "Mass Spectrometric Analysis of Adducts of Sulfur Mustard Analogues to Human Plasma Proteins: Approach towards Chemical Provenancing in Biomedical Samples." *Analytical and Bioanalytical Chemistry* 413, no. 15 (April 26, 2021): 4023–36. https://doi.org/10.1007/s00216-021-03354-z.

Holmgren, Karin Höjer, Hanna Hakulinen, Rikard Norlin, Mirjam de Bruin-Hoegée, Marie Spiandore, Samantha Qi See, Renee Webster, et al. "Interlaboratory Comparison Study of a Chemical Profiling Method for Methylphosphonic Dichloride, a Nerve Agent Precursor." *Forensic Chemistry* 33 (May 2023): 100473. https://doi.org/10.1016/j.forc.2023.100473.

Säde, Solja, Grégoire Delaporte, Carlos G. Fraga, Hanna Hakulinen, Karin Höjer Holmgren, Marie Spiandore, Crister Åstot, et al. "Interlaboratory Development and Proposition for a New Quality Control Sample for Chemical Forensics Analysis of Chemical Warfare Agents." *Talanta Open* 8 (December 2023): 100249. https://doi.org/10.1016/j.talo.2023.100249.

Vanninen, Paula. Recommended operating procedures for analysis in the verification of chemical disarmament. Helsinki, Finland: University of Helsinki, 2023.

#### 10. AGENDA ITEM TEN – Privacy-enhancing technologies in data and AI systems

- 10.1 Dr Thierry Rakotoarivelo from the Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia, provided an overview of the work of the Privacy Technology Research Group, which is part of Data61. He opened his presentation with a description of Data61—a data and digital innovation research and development organisation within CSIRO. Data61 has three research capabilities, and the Privacy Technology Research Group sits in the software and computational systems capability, which aims to increase the responsible, secure, and safe adoption of emerging digital technologies in Australian organisations and communities.
- 10.2 In the first part of the presentation, Dr Rakotoarivelo focused on the research and technologies that the Privacy Technology Research Group has been developing to measure and assess privacy and sensitive information issues in data and AI systems. He highlighted three case studies on quantitative privacy risk measurements (specifically risk of re-identification), qualitative risk assessments, and emerging privacy challenges with large language models.
- 10.3 In the second part of his presentation, Dr Rakotoarivelo provided an overview of the methods being developed in the Privacy Technology Research Group for controlling privacy risks within an acceptable range for data custodians. He highlighted two key points from this work. First, there are trade-offs when designing privacy risk mitigations to balance objectives such as privacy, utility, fairness, transparency, and explainability. Second, privacy-enhancing mechanisms are one of the approaches used to manage privacy, and a given privacy/utility balance may be achieved through different combinations of factors such as regulation, technology, and access control.
- 10.4 Finally, Dr Rakotoarivelo presented three detailed examples of privacy-enhancing technologies researched and developed by the Privacy Technology Research Group. The first was a mechanism to generate privacy-preserving synthetic tabular multidimensional data, which accurately captures and represents the two- and three-way correlations that exist in the original data. The second introduced work done by private query release, private and fair data linkage, and private federated learning. The last example focused more closely on the trade-offs between privacy and fairness. It demonstrated how privacy enhancements in ML models impact the fairness of their predictions, and conversely, how fairness-enhancing approaches in ML model training impact the vulnerability of these models to information leakage during inference time.
- 10.5 Members of the TWG commented on several topics mentioned by Dr Rakotoarivelo and focused on privacy, model reliability, and biases in particular. It was highlighted that increased privacy can lead to decreased reliability of AI models. Dr Rakotoarivelo noted that biases in the underlying data can impact the accuracy of the final model, but that there are various approaches that can be applied to overcome this, including repartitioning the training dataset, collecting more diverse datasets, and using reinforcement learning. Dr Rakotoarivelo also discussed trade-offs between applying privacy-preserving mechanisms centrally or locally.

## 11. AGENDA ITEM ELEVEN – Breakout sessions – Subgroups 1 and 2 (together) and Subgroups 3 and 4 (together)

See agenda item 2.

#### 12. AGENDA ITEM TWELVE – Group discussion

See agenda item 2.

#### 13. AGENDA ITEM THIRTEEN – Closing remarks and any other business

In closing, the Chairperson and Vice-Chairperson outlined the timing and frequency of their drafting meetings over the coming months and urged the TWG members to continue to review and contribute to the text, recalling that the end-of-mandate report is a collective endeavour and must be agreed by consensus. Dr Bossée thanked the TWG members and external speakers for their contributions and discussions and noted that significant progress had been made. She also expressed her thanks to Dr Hakulinen for hosting the fifth TWG meeting at VERIFIN. No additional points were raised.

### 14. AGENDA ITEM FOURTEEN – Closure of the meeting

The Chairperson closed the meeting at 16:09 (CET) on 13 June 2025.

#### **ACKNOWLEDGEMENTS**

The TWG members thank the guests and members of the Secretariat who participated in discussions. The TWG is very grateful to Dr Hakulinen and VERIFIN for hosting and supporting the fifth TWG meeting in Finland. The TWG also wishes to acknowledge Ms Ernesa Ademagić of the OPCW Office of Strategy and Policy for her support and contributions to the meeting and its preparations. Lastly, the TWG thanks the OPCW Director-General for his establishment and support of the TWG, and acknowledges the generous contributions of the European Union and the United States of America that help to cover the costs of the Group's work.

Annex: List of Participants at the Fifth Meeting of the Scientific Advisory Board's Temporary Working Group on Chemical Forensics

#### Annex

# LIST OF PARTICIPANTS AT THE FIFTH MEETING OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP ON CHEMICAL FORENSICS

	Participant	Institution
1.	Prof. Arian van Asten	University of Amsterdam, Netherlands
2.	Dr Crister Åstot*	Swedish Defence Research Agency (FOI), Sweden
3.	Capt. Elma Biscotti*	Scientific and Technical Research Institute for
		Defense (retired), Argentina
4.	Dr Anne Bossée*	DGA CBRN Defence, France
	(Chairperson of the TWG)	
5.	Dr Grégoire Delaporte	DGA CBRN Defence, France
6.	Ms Anne-Marie Fortin	United Nations Office on Drugs and Crime,
		International
7.	Dr Hanna Hakulinen	Finnish Institute for Verification of the Chemical
	NA T II '	Weapons Convention (VERIFIN), Finland
8.	Ms Ang Lee Hwi	DSO National Laboratories, Singapore
9.	Prof. Imee Su Martinez*	University of the Philippines Diliman, Philippines
10.	Dr Simon Ovenden	Defence Science and Technology Group, Australia
11.	(Vice-Chairperson of the TWG)  Dr Meehir Palit*	Defense Bessenh and Development Opposition
11.	Dr Meenir Pant	Defence Research and Development Organisation, India
12.	Col. Günter Povoden	CBRN Defence Centre, Austrian Armed Forces,
12.	Con. Gunter 1 ovoden	Austria
13.	Dr Sarah Stubbs	Defence Science and Technology Laboratory (Dstl),
		United Kingdom of Great Britain and Northern Ireland
14.	Dr Hongmei Wang	State Key Laboratory of NBC Protection for Civilian,
		China
15.	Dr Audrey Williams	Lawrence Livermore National Laboratory, United
		States of America
	Invited Speakers	Institution
16.	Dr Cornelia Rasmussen	University of Texas at Austin, United States of
1.7	B C C . *	America
17.	Prof. Sermet Sezigen*	University of Health Sciences, Türkiye
18.	Dr Anders Nordgaard	Swedish National Forensic Centre, Sweden
19.	Dr Maria Wallenius	Joint Research Centre, European Commission
20.	Dr Carlos Fraga	Air Force Research Laboratory, United States of
21	Da Thiomy Dolote arival	America  Commonwealth Scientific and Industrial Research
21.	Dr Thierry Rakotoarivelo	Organisation (CSIRO), Australia
	Technical Secretariat Staff	Division
22.	Dr Peter Hotchkiss	Office of Strategy and Policy
	(Secretary to the SAB)	Office of Strategy and Folicy
	(Sectionary to the DAD)	

<sup>\*</sup> Member of the SAB.