OPCW

Scientific Advisory Board

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SUMMARY OF THE FIRST MEETING OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP ON CHEMICAL FORENSICS 25 AND 26 MARCH 2024

1. AGENDA ITEM ONE – Opening of the meeting

1.1 The Temporary Working Group (TWG) on Chemical Forensics of the Scientific Advisory Board (SAB) held its first meeting on 25 and 26 March 2024 in a virtual format via videoconferencing. The meeting was chaired by Dr Anne Bossée on behalf of the SAB, with Dr Simon Ovenden as Vice-Chairperson.

1.2 This first official meeting of the TWG followed an initial informal meeting that took place in January, shortly after the start of the Group's mandate. At this meeting, the SAB Secretary provided a brief overview of the OPCW's establishment and mandate, as well as of provisions related to the establishment of the SAB and related temporary working groups, as provided by the SAB terms of reference. He also commented on aspects of operation of the TWG to include points of contact, file storage and sharing, and reporting requirements. The TWG Chairperson provided an overview of the terms of reference and composition of the TWG, which are detailed in Annexes 1 and 2 hereto, respectively.

1.3 Dr Bossée opened this first official meeting by welcoming TWG members and expressing her pleasure and honour to be chairing this TWG, with Dr Ovenden as the Vice-Chairperson. As no objections or comments were raised in response to the proposed programme of work during the two days of the meeting, the agenda was adopted.

2. AGENDA ITEM TWO – Adoption of the agenda

The TWG adopted the following agenda for its first meeting:

1. Opening of the meeting
2. Adoption of the agenda
3. Presentation from the OPCW Laboratory
4. Chemical weapons: Status of forensic technologies and challenges to source attribution
5. Update on the Chemical Forensics International Technical Working Group
6. Chemical forensics approaches

7. Subgroup breakout sessions

8. General discussion

9. Final comments and next steps

10. Closure of the meeting

3. AGENDA ITEM THREE – Presentation from the OPCW Laboratory

3.1 The Head of the OPCW Laboratory, Dr Daan Noort, opened his presentation with a brief overview of the key tasks undertaken at the Laboratory, namely providing support to sampling and analysis, maintaining ISO 17025 and ISO 17043 standard accreditation, and providing capacity-building training courses to States Parties. He emphasised that sampling and analysis provides factual evidence for the presence or absence of scheduled chemicals and underpins the verification regime.

3.2 Dr Noort explained that, particularly in terms of authentic samples, very little analysis is performed at the OPCW Laboratory, as this is the work of the network of designated laboratories. He then explained the two types of designated laboratory, and reported that, as of February 2024, there are 26 designated laboratories in 21 States Parties for the analysis of environmental samples, and 19 designated laboratories in 14 States Parties for the analysis of biomedical samples. Of these, a total of 15 laboratories are designated for the analysis of both environmental and biomedical samples. Finally, Dr Noort outlined the proficiency test process used to test the competencies of the designated laboratories on an annual basis.

3.3 Prior to 2013, no authentic samples had ever been received by the network of designated laboratories. This changed following the use of chemical weapons in the Syrian Arab Republic and the subsequent establishment of three non-routine missions: the Declaration Assessment Team in 2014; the OPCW Fact-Finding Mission in Syria in 2014; and the Investigation and Identification Team (IIT) in 2018. Chemical forensics techniques have been critical to the work of the IIT, in particular. Dr Noort highlighted a recent example from the fourth report of the IIT (S/2255/2024, dated 22 February 2024) relating to samples from a 2016 incident that were collected in 2021. Chemical forensics techniques were leveraged to identify numerous sulfur mustard degradation products and synthesis by-products—especially multi-sulfur chemicals—present in samples collected, enabling the sulfur mustard's production route to be confirmed as the Levinstein synthesis process. Furthermore, the presence of polychlorinated sulfur mustard analogues was important for determining the perpetrators of the chemical weapons attack, as the mustard was produced by an improvised method. This highlighted the importance of having the ability to identify degraded samples and degradation routes, given the challenges associated with acquiring samples from security-risk areas and in complex political environments that may hinder timely sample collection.

3.4 To ensure that designated laboratories are fit for purpose in terms of chemical forensics, four key areas have been identified for technical development: reporting and probabilistic interpretation; statistical processing and feature comparison; data processing methods and quality control; and quantitative analysis and measurement uncertainty. Owing to the difficulties in shipping test samples containing intact agent,

a series of "dry" laboratory exercises have been proposed, where raw data of sample or data sample sets will be sent to participants instead. Traditional "wet" exercises will continue in parallel, with an emphasis on quantification of the analytes. In the proficiency tests, there is currently no requirement to quantify the reported chemicals, only to confirm the presence or absence of the analytes.

3.5 There are currently two chemical forensics research projects being undertaken at the OPCW Laboratory. The first aims to develop chemical forensics analytical methods with an application beyond scheduled chemicals based on stable light isotope analysis of chlorine and sulfur. This work will be critical for production route attribution, sample matching, and the identification of discriminating markers. The second project also aims to develop chemical forensics analytical methods using inductively coupled plasma-tandem mass spectrometry (ICP-MS/MS), with a specific focus on the analysis of biotoxins. This will lead to attribution of the geographical origin of biotoxins, as well as elucidation of production or isolation techniques.

3.6 The availability of reference standards, particularly for non-traditional agents, is fundamental to the effective application and exploitation of chemical forensics techniques. In light of this, the new OPCW Centre for Chemistry and Technology includes a state-of-the-art microsynthesis facility where such reference standards may be produced. This will support the development of investigative science and technology at the OPCW Laboratory and ensure evidence-based advice can be provided to the Technical Secretariat (the Secretariat) at short notice. Wet chemistry—initially for the synthesis of non-toxic materials—is planned to start by the end of 2024.

3.7 Dr Noort concluded his presentation by stating that collaboration between the OPCW Laboratory and designated laboratories will be crucial for the success of this endeavour. He also highlighted a number of capabilities that, in his view, need to be considered, including synthesis knowledge from organic chemists, quantitative analysis, trace analysis, probabilistic models, and a repository of reference standards, among others.

3.8 Following Dr Noort's presentation, TWG members posed a number of questions and discussed various issues. They recognised the important collaboration required between organic and analytical chemists, while they also considered the ability to share synthesis data, and highlighted the sensitivities around this. It was noted that the reporting requirements for chemical forensics work will be distinctly different to those of traditional proficiency tests. Consequently, significant work will be required by the OPCW in order to develop a suitable reporting format for unscheduled chemicals at trace levels for future chemical forensics exercises. Trace analysis was optional and therefore rarely performed in previous proficiency tests, but it will be an integral part of dedicated chemical forensics exercises. Dr Noort made clear that the application of chemical forensics approaches is not restricted to traditional scheduled chemicals, and that the chemical landscape is unpredictable. Finally, computational models were briefly discussed. It was acknowledged that such models are particularly useful in the field of chemical forensics, but communication of their use requires careful consideration to ensure that they are trusted and not perceived as a poorly understood "black box" by investigators or in court.

4. AGENDA ITEM FOUR – Chemical weapons: Status of forensic technologies and challenges to source attribution

4.1 The United States Government Accountability Office (GAO) is an independent, non-partisan agency that provides fact-based information that can be used to improve government and save taxpayers billions of dollars. GAO has a science and technology portfolio. It is within this context, explained Dr Karen Howard, the Director of Science, Technology Assessment, and Analytics at GAO, that they embarked on a study to assess the status of technologies available to identify a chemical agent or its source, in regard to chemical weapons, and describe challenges and relevant policy options. The study was published and made available to the public in September 2023.[1]

4.2 A multifaceted approach was taken to collect pertinent information and to include an in-depth review of the literature, interviews, and meetings with experts in the field, as well as site visits to laboratories where chemical weapons-related chemical forensics research was taking place. Four discrete steps were identified in any chemical forensics investigation, from incident to final analysis: sample collection; sample preparation; instrumental analysis; and data interpretation. Dr Howard highlighted the fact that many of the technologies used for identifying chemical agents are fairly mature, despite often having some limitations. However, methods based on chemical analysis that are used to provide information about a chemical agent's history are still mostly under development.

4.3 Dr Howard identified a number of challenges to chemical identification and attribution, including sample quantity and quality, limited or incompatible reference data, limited information sharing due to sensitivities, and hindered improvements to methods and technology. She reiterated Dr Noort's point that sample degradation may occur owing to delayed access to the incident scene, and highlighted that this may also arise as a result of logistical issues. Shortening the time between sampling and off-site analysis would reduce the degradation of intact chemicals, minimising the number of chemical agent signatures generated. To conclude, Dr Howard outlined several policy options, emphasising the opportunities and challenges each pose.

4.4 The ensuing discussion with the TWG members focussed on the availability of data. Namely, how existing data in incompatible formats, such as hard copies of raw data and spectra, could be added to electronic data, potentially creating a new database, and how different governments' priorities and sensitivities could be overcome in order to better share data and information.

5. AGENDA ITEM FIVE – Update on the Chemical Forensics International Technical Working Group

5.1 Dr Katie McCormac-Miller, a physical scientist in the Bureau of Arms Control, Deterrence, and Stability at the United States Department of State, provided an overview of the history and current status of the Chemical Forensics International Technical Working Group (CFITWG).

5.2 The CFITWG was established in 2017 to address gaps in chemical forensics research and development, and is an ad hoc, voluntary association of chemical forensics

[1] https://www.gao.gov/assets/gao-23-105439.pdf.

practitioners. It consists of experts from a variety of institutions, including members of the OPCW, OPCW designated laboratories, government laboratories, academia, the law enforcement community, and export control organisations.

5.3 The CFITWG looks to enhance partnerships and collaboration, and to identify and prioritise scientific gaps in four different priority areas of research—namely, profiling and provenance of chemicals; databases and interpretation for sourcing chemicals; chemometrics, data analysis, and interpretation; and the chemical forensic investigative chain.

5.4 The Office of Chemical and Biological Weapons Affairs within the Bureau of Arms Control, Deterrence, and Stability in the United States Department of State is currently leading the CFITWG effort, with meetings held twice a year. The next meeting will take place on the margins of the chemical forensics session at the American Chemical Society Fall 2024 national meeting in Denver, Colorado.

5.5 There was notable support for the work of the CFITWG by TWG members. The meetings provide a valuable forum for experts in the community to discuss relevant progress in the field, while the recent multi-laboratory profiling exercise was considered particularly successful.[2] Maintaining the informal nature of the CFITWG was strongly encouraged, and current and potential sources of funding for the Group were also discussed.

6. AGENDA ITEM SIX – Chemical forensics approaches

6.1 Prof Arian van Asten highlighted the current research in the field of forensic analytical chemistry and on-scene chemical analysis being conducted by his group at the University of Amsterdam. Their research focuses on three main areas—namely, illicit drugs; explosives; and chemical warfare agents (CWA). In terms of illicit drugs and explosives, recent emphasis has been placed on rapid chemical identification and exploring and leveraging the enhanced capabilities afforded by incorporating data science and chemometric approaches. One interdisciplinary approach is combining the expertise of chemists, data scientists, and criminologists to mine the analytical data from illicit drug screening and determine what additional information can be deduced.

6.2 Prof van Asten recognised that CWA pose additional challenges compared to illicit drugs and explosives. These may include limited or no access to an incident site and highly reactive chemicals that degrade rapidly. Within the Van Asten group, various aspects of a forensic reconstruction of an incident involving CWA have been examined. Dried blood spots have been explored and determined to be a viable alternative to whole blood samples, and have a number of advantages, including being stable over long periods of time.[3]

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[2] Karin Höjer Holmgren, Hanna Hakulinen, Rikard Norlin, Mirjam de Bruin-Hoegée, Marie Spiandore, Samantha Qi Shu See, Renee Webster, et al. 2023. “Interlaboratory Comparison Study of a Chemical Profiling Method for Methylphosphonic Dichloride, a Nerve Agent Precursor.” Forensic Chemistry, Vol. 33 (May 2023), pp. 100473–1004. doi:10.1016/j.forc.2023.100473.

[3] Mirjam de Bruin-Hoegée, Alex Fidder, Tomas van Groningen, Marcel J. van der Schans, Daan Noort, and Arian C. van Asten. 2023. “On-Site Detection and Laboratory Verification of the Presence of Nerve Agent Biomarkers Using Dried Blood Spots.” Forensic Chemistry Vol. 35 (September 2023), pp. 100526–100534. doi:10.1016/j.forc.2023.100526.

6.3 Biomarkers for chemical exposure have also been identified. While the detection of chlorinated adducts of the amino acid tyrosine, which is released by pronate digestion of human proteins, may indicate exposure to chlorine, inflammatory responses in the body may also produce a background of such chlorinated tyrosine adducts. Consequently, the Van Asten group has focussed on protein markers, such as chlorination products of peptides, and a number of promising peptides have been identified. The plant biomarker work, conducted under the OPCW Plant Biomarker Challenge, identified useful biomarkers for exposure to chlorine and other CWA including nerve agents.[4,5] Initial work has shown that the biomarkers are not plant-dependent and are stable in plant material for at least three months post-exposure.

6.4 In an innovative study, the Van Asten group has explored the feasibility of determining additional information about illicit drugs after being metabolised in the body.[6] Fentanyl was synthesised by both the Gupta and Siegfried routes and the resultant samples were exposed to a liver-cell system to mimic metabolism. Having employed a data analysis approach based on liquid chromatography-high resolution mass spectrometry (LC-HRMS) and chemometrics, it was confirmed that the synthesis routes of the fentanyl samples could be distinguished post-metabolism.

6.5 The group's research is not only focussed on CWA but also on related aspects such as dissemination devices, which may provide additional insights into an incident. Laser ablation inductively coupled plasma-mass spectrometry (LA-ICP-MS) is a versatile analytical technique that may be used in the forensic examination of glass, and a number of high-quality standards are available. The Van Asten group has explored this technique's applicability to the forensic examination of polymers, a common material in dissemination devices. In collaboration with the National Institute of Standards and Technology (NIST), new polymer standards have been developed, leading to the subsequent development of an 18-element attribution signature for plastic materials.[7] This approach was then applied to a wide range of plastic objects procured from the United States of America and within the European Union. Not only could the source of the polymers be attributed, but application of data analysis techniques also enabled the polymer classification (tape, tubing, wire) to be determined, which is particularly useful when only traces remain at the incident scene.

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4 Mirjam de Bruin-Hoegée, Latifa Lamriti, Jan P. Langenberg, René C. M. Olivier, Lai Fum Chau, Marcel J. van der Schans, Daan Noort, and Arian C. van Asten. 2023. "Verification of Exposure to Chemical Warfare Agents through Analysis of Persistent Biomarkers in Plants". Analytical Methods Vol. 15 (January 2023), pp. 142 – 153. doi:10.1039/d2ay01650h.

5 Mirjam de Bruin-Hoegée, Irene M. van Damme, Tomas van Groningen, Debora van der Riet-van Oeveren, Daan Noort, and Arian C. van Asten. 2022. "Elucidation of In Vitro Chlorinated Tyrosine Adducts in Blood Plasma as Selective Biomarkers of Chlorine Exposure." Chemical Research in Toxicology Vol. 35 (6), pp. 1070–1079. doi:10.1021/acs.chemrestox.2c00053.

6 Mirjam de Bruin-Hoegée, Djarah Kleiweg, Daan Noort, and Arian C. van Asten. 2021. "Chemical Attribution of Fentanyl: The Effect of Human Metabolism." Forensic Chemistry Vol. 24 (June 2021), pp. 17950–17958. doi:10.1016/j.forc.2021.100330.

7 Mirjam de Bruin-Hoegée, Jorien Schoorl, Peter Zoon, Marcel J. van der Schans, Daan Noort, and Arian C. van Asten. 2023. "A Novel Standard for Forensic Elemental Profiling of Polymers by LA-ICP-TOF-MS." Forensic Chemistry Vol. 35 (September 2023), pp. 100515–100525. doi:10.1016/j.forc.2023.100515.

6.6 The most recent projects include developing a disposable near-infrared sample container that could be used for instantaneous identification of liquid CWA in the field. The Van Asten group is also considering how data from different spectroscopic techniques (near-infrared, infrared, and Raman) could be effectively and meaningfully combined through novel data fusion concepts. Lastly, there is interest in determining the toxicity of unknown chemical compounds directly from in-field mass spectrometry detection, avoiding the need for a chemical identification step.[8]

6.7 The TWG members were keen to understand more about the interdisciplinary project which, through data mining, aims to derive additional information about illicit drug samples directly from analytical data. Prof van Asten explained that in the Netherlands approximately 25,000 drug samples are screened annually by customs, the police, and the Netherlands Forensic Institute. Given the high numbers of samples, the emphasis is on speed and efficiency and the aim is to produce a clean spectrum of the compound of interest—a particular illicit drug—that can be used in an investigation. The data files contain a lot of additional information about the sample, such as adulterants and impurities, but this is often not exploited as part of the forensic process. The Van Asten group is exploring what additional information can be extracted from these data and is looking to automate the process and conduct it in real time with the chemical analysis. An understanding of the information that can be extracted could be valuable in the context of CWA incidents. This is especially important as there are considerably fewer samples and sensitivities around data sharing. Prof van Asten emphasised that this data science approach is very different to a traditional chemistry-centric one. The group is currently establishing the realm of the possible and recognises that there will be limitations and challenges, not least the presence of biological matrices.

7. AGENDA ITEM SEVEN – Subgroup breakout sessions

7.1 In a similar approach to previous TWGs, the Chairperson and the Vice-Chairperson decided that the work of this TWG should be broken down into four separate subgroups. This would ensure an efficient approach and a fair division of the workload. At future meetings of the TWG, subgroup leads will present the work of their respective subgroups, enabling everybody to gain insight and provide additional input into all four subgroups.

7.2 An outline of the four subgroups for this TWG is as follows:

(a) Subgroup 1, led by Dr Crister Åstot, will focus on the state of the art of chemical forensics and will address questions 6(a), 6(b) and 6(c) of the terms of reference (Annex 1). In answering these questions, subgroup members will consider the areas of batch-matching, impurity profiling, synthesis route, geographic and environmental factors, and isotope ratios:

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

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[8] Saer Samanipour, Jake W. O'Brien, Malcolm J. Reid, Kevin V. Thomas, and Antonia Praetorius. 2023. "From Molecular Descriptors to Intrinsic Fish Toxicity of Chemicals: An Alternative Approach to Chemical Prioritization." Environmental Science & Technology Vol. 57 (46), pp. 17950–17958. doi:10.1021/acs.est.2c07353.

(ii) Can analysis of other materials that may be found, such as a storage container, or parts of a dissemination device, yield relevant information compared to liquid and soil samples?
(iii) What information is available related to the ability to conduct chemical forensics analysis on non-traditional agents which could be applied to CWA? Are there any restrictions or limitations?

(b) Subgroup 2, led by Dr Grégoire Delaporte, will focus on future capabilities addressing questions 7(a), 7(b) and 7(c) of the terms of reference, considering the analysis of large or limited datasets, dataset creation or expansion, and model validity:

(i) What impact will the increased power and integration of machine learning and deep learning have on the field of chemical forensics?
(ii) What impact will the limited size of datasets available have on CWA forensic analysis?
(iii) What will the field look like in 5 – 10 years, particularly in regard to the capabilities around the specific areas mentioned in 6?[9]

(c) Subgroup 3, led by Ms Ang Lee Hwi, will focus on methods and procedures, addressing questions 8(a), 8(b), 8(c), 8(d), 8(e) and 8(f) of the terms of reference:

(i) How can applied analytical methods have an impact on the results related to trace analysis and the chemical footprint?
(ii) How can data, methods, and procedures to conduct the in-depth CWA analyses expected in chemical forensics be standardised and shared?
(iii) What information is needed to ensure trust and reproducibility in the analysis and the results?
(iv) How can analytical data from different techniques (e.g., GC-MS, LC-HRMS and NMR)[10] be combined in forensic analysis?
(v) Would curated/shared database(s) of relevant reference data be useful? Are there any recommendations/restrictions to secure these types of database(s)?
(vi) What best practices exist for on-site sampling to ensure the validity of subsequent forensic laboratory analysis and what challenges/gaps remain?

(d) Subgroup 4, led by Dr Hanna Hakulinen, will focus on the augmentation of the OPCW's capabilities by addressing questions 9(a), 9(b), 9(c), 9(d) and 9(e) of the terms of reference:

(i) How can the OPCW enhance its capability to capture and utilise chemical forensics-related information in the context of alleged use?
(ii) How will the OPCW ensure the validity of the forensic results?
(iii) How will the forensic results be reported? (criteria, level of confidence)

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9 See paragraph 6, Annex 1.

10 GS-MS = gas chromatography-mass spectrometry; NMR = nuclear magnetic resonance.

(iv) Are there other organisations or information that could be leveraged to augment the capability of the OPCW?

(v) How can forensics analysis be promoted and enhanced at Designated Laboratories? How might other organisations or laboratories contribute?

7.3 Each TWG member was asked to participate in at least one, but not more than two, of these subgroups. Time was provided on each of the two days for the subgroups to meet to discuss their initial ideas on the terms of reference on which they will focus and how to approach their work. The subgroup leads then briefed the wider TWG during the plenary general discussion session.

8. AGENDA ITEM EIGHT – General discussion

8.1 The TWG Chairperson turned the floor over to each subgroup lead in turn, to provide an overview of their subgroup and how they will consider addressing their assigned questions.

8.2 Dr Åstot reported that Subgroup 1 had begun its breakout group discussions by considering some of the challenges ahead. An important aspect of its work will be to identify relevant subfields within the broader forensic science and forensic chemistry fields where effective strategies, tools, and techniques may be leveraged. It was agreed that relevant expertise is likely to exist in the areas of environmental forensics, food analysis, metabolomics, and proteomics. Furthermore, forensic laboratories are likely to have expertise in the analysis of materials used to store or disseminate CWA, such as containers and weapon components.

8.3 The limited availability of data was highlighted and the utility of applying in silico methods to extract additional data was discussed. The legal and political aspects—including the resulting shifting time frames and increasing degradation risk—were also briefly evaluated, and the ongoing investigations into alleged CWA use in the Syrian Arab Republic were considered for closer analysis throughout the subgroup's work.

8.4 It was agreed that a detailed literature review would be required to help address the questions of Subgroup 1, and that resources can be readily accessed. Potential expert speakers, especially those in the fields of drug analysis, food analysis, and environmental chemistry, were discussed.

8.5 Dr Delaporte reported that Subgroup 2 will focus on new data analysis methods from deep learning and machine learning. It was agreed that deep and machine learning's requisite of large datasets presents a problem for the application of chemical forensics approaches to CWA, owing to the more limited datasets available. Prof van Asten commented that in silico tools would likely be the best way to address this problem. This could be achieved by creating realistic, but artificial, data by using existing data and then applying machine learning techniques, thus overcoming the issue of limited datasets. Other participants concurred with this opinion. Subgroup 2 members recognised that the potential for artificial intelligence to more easily combine and standardise datasets is also noteworthy but agreed that what datasets need to include is also a pressing concern. The importance of anonymising information for forensic legal perspectives was also recognised.

8.6 Subgroup 2 concluded that clear and precise definitions are necessary as a first step to answering the relevant questions, and that assessing the advances that adjacent fields, such as food science or environmental sciences, have made in chemical analysis will be crucial.

8.7 There was wider agreement amongst the TWG members that a set of agreed definitions for all key terms is required. The report from the TWG on Investigative Science and Technology contains a glossary of terms and this will be consulted and developed appropriately.

8.8 Ms Ang reported that Subgroup 3 discussed methods and procedures relevant to chemical forensics with a view to building a shared database of reference materials. National security and data sensitivity concerns mean that such a database would require a custodian, a role which the OPCW could potentially fulfil. Harmonising methods and procedures—namely, standard and recommended operating procedures—would be an important task prior to collating this database, and inter-laboratory exercises are needed for standardisation and sharing of expertise. Adapted legacy data, sample matrices, existing databases, and detection profiles of dissemination technologies could also be usefully integrated into the database. Metabolomics and data fusion are other key areas of interest. Machine learning and data fusion in particular may be leveraged to combine data from different techniques. An on-site sampling protocol is also required to ensure the validity of forensic analysis. Important considerations include who is authorised to perform collection of samples, and collection of background samples to counteract matrix effects which affect the level of impurities. Existing guidelines for nuclear forensics and the Generic Integrated Forensic Toolbox for CBRN incidents project—a European capability project which ran from 2014 to 2017—may be sources of inspiration.[11] Making use of other chemical forensics laboratories and anticipating the impact of machine learning and artificial intelligence on chemical forensics were raised in this discussion.

8.9 Dr Simon Ovenden, on behalf of Dr Hakulinen, reported that Subgroup 4 had discussed pathways to augment the OPCW's capabilities in forensic chemistry. In the context of question 9(e), the prospect of gathering forensic chemistry expertise from organisations and laboratories outside the network of designated laboratories was explored. External expertise may prove highly useful but has limitations and should complement agent chemistry expertise from designated laboratories. The relative benefits and shortcomings of proficiency tests and confidence-building exercises were examined with an understanding of the time and resource intensive nature of chemical forensic activities.

8.10 All four subgroups confirmed plans to meet virtually in early to mid-May.

[11] For more information on the Generic Integrated Forensic Toolbox for CBRN incidents project, see: .

9. AGENDA ITEM NINE – Final comments and next steps

9.1 The TWG Chairperson commended the members on a very productive first meeting and invited them to work on their respective questions and to meet during the intersessional period, with a view to presenting preliminary results of their deliberations, including the agreed approach, in the second meeting of the TWG, scheduled from 3 to 5 June 2024 as an in-person meeting.

9.2 It was agreed that the third meeting of the TWG would take place, in person, in the autumn and the dates would be agreed by correspondence.

10. AGENDA ITEM TEN – Closure of the meeting

The Chairperson ended the meeting at 16:00 (CET) on 26 March 2024.

ACKNOWLEDGEMENTS

The TWG members thank the guests and members of the Secretariat who participated in discussions. 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 contribution of the European Union that helps to cover the costs of the Group's work.

Annexes:

Annex 1: Terms of Reference of the Scientific Advisory Board's Temporary Working Group on Chemical Forensics

Annex 2: List of Participants at the First Meeting of the Scientific Advisory Group's Temporary Working Group on Chemical Forensics

Annex 1

TERMS OF REFERENCE OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP ON CHEMICAL FORENSICS

1. The threat of use of chemical weapons remains. However, the ways in which chemicals may be used as weapons is evolving. While the threat that chemical weapons may be misused by a State actor in a large-scale attack still exists, there is growing concern around other scenarios of misuse of chemicals, such as by non-State actors as well as more targeted uses by States. In addition, there is an increasing potential for non-traditional agents to be used. These include biotoxins and central nervous system-acting chemicals, among others. Given the expanding threat spectrum, and the myriad attack uses and scenarios, it is more important than ever that as much information as possible be derived from any available samples from an alleged attack. It is imperative that the OPCW be able to fully understand and harness the utility of chemical forensics approaches and be able to use validated results in any investigation of misuse of a chemical.

2. In order to strengthen and augment the Technical Secretariat's capability in this regard, an in-depth review of the methods and technologies used in the field of chemical forensics would be a particularly valuable exercise and highly relevant in the current threat landscape. Further to his response to the report of the Thirty-Seventh Session of the Scientific Advisory Board (SAB), (EC-104/DG.22, dated 27 September 2023) and in accordance with paragraph 9 of the terms of reference of the SAB (Annex to C-II/DEC.10/Rev.1, dated 2 December 2004), the Director-General has decided to establish a Temporary Working Group (TWG) on Chemical Forensics and has appointed Dr Anne Bossée as the Chairperson of the Group.

3. The objective of the TWG is to review the science and technology relevant to chemical forensics and identify remaining gaps and challenges such that the OPCW can make best use of the information chemical forensics can yield moving forward. Considerations should be given to the work and recommendations from the SAB's previous TWG on Investigative Science and Technology (SAB/REP/1/19, dated 1 December 2019) as well as ongoing work in this area within the Secretariat. The findings will be considered by the SAB and recommendations will be provided to the Director-General.

4. The TWG will consist of individuals who have expertise in: chemical forensics, analysis, and/or synthesis; OPCW proficiency tests; in-field sampling; machine learning; or experience of implementation of the Chemical Weapons Convention. The TWG will comprise qualified members of the SAB as well as representatives from relevant academic, scientific and international organisations. Guest speakers will be invited regularly to assist the TWG in its collection of data and information, and formulation of advice. The TWG may also, when necessary, draw upon the expertise of the Technical Secretariat, in particular the OPCW Laboratory, Inspectorate, and non-routine missions.

5. The TWG will report to the SAB, and will address specific questions relating to four subtopics, detailed below.

6. **State of the art.** Considering these specific areas:

- Batch-matching (correlating different samples to the same production batch and the influence of matrices)
- Impurity and trace element profiling (determining the trace impurities in a sample)
- Synthesis route (deriving the synthesis route used to make a specific chemical in a sample)
- Geographic context (pinpointing a geographic area where a sample was created or stored)
- Environmental factors and storage conditions (determining whether a sample was exposed to a certain environment, such as extreme heat or cold, dust or humidity)
- Isotope ratio techniques (specifically related to phosphorus, carbon, and deuterium)

a. What is the current state of the art related to determining the life cycle of a given chemical sample?
b. Can analysis of other materials that may be found, such as a storage container, or parts of a dissemination device, yield relevant information compared to liquid and soil samples?
c. What information is available related to the ability to conduct chemical forensics analysis on non-traditional agents which could be applied to CWA? Are there any restrictions or limitations?

7. **Future capabilities**. Considering the following:

- The ability to analyse large datasets
- The ability to analyse limited datasets and the impact on model validity
- The ability to create or expand datasets to train models
- Targeted research based off data and results that have been optimised with computer models

a. What impact will the increased power and integration of machine learning and deep learning have on the field of chemical forensics?
b. What impact will the limited size of datasets available have on CWA forensic analysis?
c. What will the field look like in 5 – 10 years, particularly in regard to the capabilities around the specific areas mentioned in 6?

8. **Methods and procedures**.

a. How can applied analytical methods have an impact on the results related to trace analysis and the chemical footprint?
b. How can data, methods, and procedures to conduct the in-depth CWA analyses expected in chemical forensics be standardised and shared?
c. What information is needed to ensure trust and reproducibility in the analysis and the results?
d. How can analytical data from different techniques (e.g., GC-MS, LC-HRMS and NMR) be combined in forensic analysis?
e. Would curated/shared database(s) of relevant reference data be useful? Are there any recommendations/restrictions to secure these types of database(s)?

f. What best practices exist for on-site sampling to ensure the validity of subsequent forensic laboratory analysis and what challenges/gaps remain?

9. **Augmenting the OPCW's capabilities**.

a. How can the OPCW enhance its capability to capture and utilise chemical forensics-related information in the context of alleged use?
b. How will the OPCW ensure the validity of the forensic results?
c. How will the forensic results be reported? (criteria, level of confidence)
d. Are there other organisations or information that could be leveraged to augment the capability of the OPCW?
e. How can forensics analysis be promoted and enhanced at Designated Laboratories? How might other organisations or laboratories contribute?

10. In addition, the TWG will provide advice, as requested, on Technical Secretariat proposals for methodologies, procedures, technologies, and equipment for chemical forensics.

11. The Director-General might pose other relevant questions to the TWG, through the SAB.

12. The TWG will exist for a period of two years starting 1 January 2024. Thereafter, its work will be reviewed by the SAB and the Director-General, and a decision will be made as to whether it should continue its work and, if so, whether these terms of reference should be revised.

Annex 2

LIST OF PARTICIPANTS AT THE FIRST 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 Khaldoun Bachari	Center for Scientific and Technical Research in Physical and Chemical Analysis (CRAPC), Algeria
3	Capt Elma Biscotti*	Scientific and Technical Research Institute for Defense, Argentina
4	Dr Anne Bossée* (Chairperson of the TWG)	DGA CBRN Defence, France
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 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 (Vice-Chairperson of the TWG)	Defence Science and Technology Group, Australia
11	Dr Meehir Palit*	Defence Research and Development Organisation, India
12	Mr Günter Povoden*	CBRN Defence Centre, Austrian Armed Forces, Austria
13	Dr Sarah Stubbs	Defence Science and Technology Laboratory, United Kingdom of Great Britain and Northern Ireland
14	Dr Hongmei Wang	State Key Laboratory of NBC Protection for Civilians, China
15	Dr Audrey Williams	Lawrence Livermore National Laboratory, United States of America
16	Dr Crister Åstot*	Swedish Defence Research Agency (FOI), Sweden
	External Speakers	**Institution**
17	Dr Karen Howard	United States Government Accountability Office
18	Dr Katie McCormac-Miller	Bureau of Arms Control, Deterrence, and Stability, United States Department of State
	Technical Secretariat Staff	**Division**
19	Dr Peter Hotchkiss (Secretary to the SAB)	Office of Strategy and Policy
20	Dr Daan Noort	OPCW Laboratory

* Member of the SAB.

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