OPCW

Scientific Advisory Board

Thirty-Sixth Session
26 – 29 September 2022

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REPORT OF THE SCIENTIFIC ADVISORY BOARD AT ITS THIRTY-SIXTH SESSION

1. AGENDA ITEM ONE – Opening of the session

1.1 The Scientific Advisory Board (SAB) met for its Thirty-Sixth Session from 26 to 29 September 2022. The session was chaired by Mr Günter Povoden, with Dr Andrea Leisewitz serving as Vice-Chairperson.

1.2 Mr Povoden opened the Thirty-Sixth Session of the SAB by welcoming the SAB members and reminding the Board of the work ahead, highlighting the need to finalise the Board's report on developments in science and technology for the Fifth Review Conference.[1] The SAB Chairperson also welcomed the invited speakers and noted that he was looking forward to their presentations and the discussions that followed.

Executive summary

1.3 The Board met in person at the OPCW Headquarters for the second time in 2022. This second meeting was important for the Board to continue its work on the report to the Fifth Review Conference. Most Board members were able to travel for the meeting, though those who could not were able to participate virtually via the Organisation's video conferencing equipment.

1.4 The main focus of the session was finalising the Board's report to the Fifth Review Conference. This involved a number of in-session meetings by the subgroups focusing on different scientific topics of relevance to the Chemical Weapons Convention (hereinafter "the Convention"). During a plenary session, the SAB also deliberated on the entire list of recommendations that it wants to make in its report, ensuring consensus among all its members. In addition, the Board was able to take a guided tour of the Centre for Chemistry and Technology (ChemTech Centre). Although construction continues, the Board was very impressed with the size, layout, and scope of the building and is excited to be able to provide advice on the future scientific activities that may be held there and contribute accordingly. The Board also heard from a number of staff members of the Technical Secretariat (hereinafter "the Secretariat"), and received updates from the SAB Secretary, the Director of Verification, the Office of Strategy and Policy, the Implementation Support Branch, the International Cooperation Branch, and the Declaration Assessment Team (DAT). In addition, the Board heard from several external speakers on topics such as chemical profiling approaches to chemical warfare

* Reissued in English for technical reasons.

1 Review Conference = Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention.

agents, studies on chemical weapons dumped at sea, and using insects as chemical samplers. Several Board members also spoke about their own research and provided updates on recent activities of interest to the SAB.

1.5 Based on the deliberations held at its Thirty-Sixth Session, the Board recommends through this report that the Director-General consider convening a topical workshop on emerging science and technology and the impact thereof on the work of the Organisation. Through its deliberations to finalise the report to the Fifth Review Conference, as well as recent topical workshops on artificial intelligence-assisted chemistry and emerging scientific trends and directions in the chemical industry, the SAB feels it is appropriate to consider a broader look at new innovations and discoveries with the aim of understanding their potential impact on the Convention and the work of the OPCW.

2. AGENDA ITEM TWO – Adoption of the agenda

The SAB adopted the following agenda for its Thirty-Sixth Session:

1. Opening of the session
2. Adoption of the agenda
3. *Tour de table*
4. Establishment of a drafting committee
5. Welcome address by H.E. Fernando Arias
6. Update on the activities of the Technical Secretariat and the Scientific Advisory Board
7. Status of research at VERIFIN[2]
8. Capacity-building programmes of the Technical Secretariat in support of the peaceful uses of chemistry under the implementation of Article XI of the Chemical Weapons Convention
9. Update on the Temporary Working Group on the Analysis of Biotoxins
10. Updates from the Verification Division
11. Scientific report to the Fifth Review Conference – Subgroup breakout discussions
12. Insects as environmental samplers
13. Interlaboratory comparison study of a chemical profiling method of methylphosphonic dichloride, a nerve agent precursor
14. Route attribution of sulfur mustard using non-targeted chemical attribution signature screening

[2] VERIFIN = The Finnish Institute for Verification of the Chemical Weapons Convention.

15. Discussion with the Declaration Assessment Team

16. Update on recent Scientific Advisory Board workshops and planning for future events

17. Discussion on central nervous system-acting chemicals

18. Update on cooperation with chemical industry associations and preparatory work for the Fifth Review Conference focusing on verification-related issues under Article VI

19. Specialised Article VI programming on verification-related issues

20. Election of the Scientific Advisory Board Chairperson and Vice-Chairperson

21. Plenary discussion on the scientific report

22. Any other business and final remarks

23. Adoption of the report

24. Closure of the session

3. AGENDA ITEM THREE – *Tour de table*

All participants in the session were invited to introduce themselves to their colleagues.

4. AGENDA ITEM FOUR – Establishment of a drafting committee

The Chairperson asked volunteers who wished to be part of the drafting committee to notify the SAB Chairperson, Vice-Chairperson, or Secretary, accordingly. Since some Board members were unable to travel to the session, it was agreed that the report would be finalised via correspondence after the session ended.

5. AGENDA ITEM FIVE – Welcome address by H.E. Fernando Arias

5.1 The Director-General of the OPCW Secretariat, H.E. Fernando Arias, welcomed everyone to the Thirty-Sixth Session of the Board. He indicated the importance of the Board's in-person meetings, though noted that technology now affords for remote participation if needed.

5.2 The Director-General reported on the progress made in the construction of the ChemTech Centre, which is nearing completion. He focused on the Secretariat's continued work in defining and developing the activities that will take place at the Centre. He commented on the complexity involved with moving the current laboratory and equipment store activities from the current location to the new ChemTech Centre, and highlighted the various aspects that will demand patience, concentration, and time. In that vein, the Director-General explained that the Secretariat plans to publish a Note describing the new and important activities that it wants to prioritise for consideration at the new Centre. He then invited the Board to take a tour of the ChemTech Centre during its session, and asked that the Board continue to discuss new, creative ideas that could be incorporated into the Centre's programming.

5.3 The Director-General noted with appreciation the recent work of the Board, from the ongoing meetings of the Temporary Working Group (TWG) on the Analysis of Biotoxins, the Board's recent topical workshops, and of course its ongoing work to prepare its report in support of the Fifth Review Conference. He reiterated the importance of the Board's report as it is essential that the Secretariat and States Parties be made fully aware of the recent developments in science and technology.

5.4 In conclusion, the Director-General thanked the Board members for their attention and wished them a productive session.

6. AGENDA ITEM SIX – Update on the activities of the Technical Secretariat and the Scientific Advisory Board

The SAB Secretary detailed the work of the Board for the session and summarised some of the important recent events and upcoming dates that the Board needs to consider. He addressed in detail the upcoming timeline of work to ensure the Board's scientific report is finished by the appropriate deadline. Last, as the International Union of Pure and Applied Chemistry (IUPAC) is holding its biennial World Chemistry Congress in August 2023 in The Hague, the SAB Secretary suggested that the Board consider holding its next in-person session either the week before or the week after this conference. Board members who are interested in participating in the conference could therefore benefit from combining both activities in one trip. Additionally, the SAB may consider how it can partner with IUPAC on some relevant activities during its conference towards promoting the work of the OPCW.

7. AGENDA ITEM SEVEN – Status of research at VERIFIN

7.1 Prof Paula Vanninen (VERIFIN) began her presentation by reminding the Board of VERIFIN's long history—not only as an OPCW designated laboratory, but also in chemical weapons research and analysis and as a partner of the OPCW in different capacity-building efforts. VERIFIN is also responsible for coordinating the publication of recommended operating procedures for analysis in the verification of chemical disarmament, what is colloquially known as the Blue Book. This compendium of procedures and analytical information is invaluable to designated laboratories and those that conduct research and analysis on chemical weapons agents. Prof Vanninen gave an update on the next edition, which is meant to be published in 2023. The Blue Book is publicly available and free to access.[3] VERIFIN also serves as the National Authority of Finland.

7.2 The presentation then turned towards the current research being conducted at VERIFIN. VERIFIN has a broad, rich suite of analytical instrumentation and developed methods that they use both in their duties as an OPCW designated laboratory for both environmental and medical samples, and for their own research interests in the area of chemical weapons verification and disarmament. In regard to research activities, VERIFIN remains very busy. It is currently engaged in several ongoing projects, including further research on newly scheduled chemicals, analysis in support of sea-dumped chemical weapons, chemical forensics, and the development of a new technology to visualise volatile chemicals.

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[3] For more information see: https://www.helsinki.fi/en/verifin/about-verifin/blue-book.

7.3 VERIFIN places importance on developing new methods and testing existing methods related to the analysis of newly scheduled chemicals (namely, entries 1.A.13 to 1.A.16 in the Annex on Chemicals to the Convention). It has an entire research team dedicated to the synthesis, samples preparation, analysis, and identification of these compounds to better understand the best ways to handle and analyse these compounds moving forward.

7.4 Sea-Dumped chemical weapons are increasingly in the spotlight as economic and environmental interests gain momentum. For example, there are numerous known sites of old, dumped chemical weapons in the Baltic Sea and the Skagerrak Strait. VERIFIN has been involved in various activities within the Chemical Munitions Search and Assessment (CHEMSEA) programme to better understand the potential existing contamination from chemical weapons dumped at sea. Since 2006, it has been analysing sediment samples from various sites and have found high concentrations of chemical weapons agent-related compounds in multiple locations. More recently, under the WARTOX programme,[4] VERIFIN has been conducting research to better understand the effects of chemical weapons on sea life. Research continues to broaden our understanding of how different bacteria may modify chemical weapons agents and associated compounds in the sea, and how these compounds impact certain species, such as water fleas and rainbow trout.[5]

7.5 VERIFIN is also heavily involved in chemical forensics work and has conducted chemical attribution analysis studies to identify synthesis by-products, impurities, degradation products, and isotopes of chemical weapons agents and related precursors to better predict synthetic pathways, the associated equipment used, and reagent sources, in addition to classifying unknown samples.[6] Of particular note, it has recently studied how impurity profiles can link source materials to intermediate synthesis products in the production of a carbamate chemical warfare agent. Much of this work is highly collaborative and involves other designated laboratories and forensics laboratories around the world.

7.6 Prof Vanninen also noted recent work on a project entitled "Gas Ion Distillation and Sequential Ion Processing Technologies for Identification and Visualization of Chemicals in Airborne Vapors (GIDPROvis)".[7] In GIDPROvis, gas ion distillation and sequential ion processing are combined to provide live visualisation of volatile chemicals in ambient environments.[8] The concept has been proven, but the maturity of the technology is still quite low. VERIFIN is working on testing the first devices and can certainly see a number of potential applications for the future, particularly in industry, but also for first responders and researchers who can then visualise chemical vapours in real time.

7.7 Upon completion of her talk, Prof Vanninen fielded several questions from the Board. Several focused on VERIFIN's work with sulfur mustard, namely the effects of DNA exposure to sulfur mustard and whether sulfur mustard conjugation products can be excreted in urine samples. Prof Vanninen noted that they have yet to look into the

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4 For more information on WARTOX see: https://www.helsinki.fi/en/verifin/tasks/research.

5 H. Niemikoski, K. K. Lehtonen, et al. Aquatic Toxicol. 241, 8, 105993 (2021). ISBN 978-951-51-8017-9.

6 N. Hamzah, M. Kjellberg, J. Chromatogr. B., et al., 1176, 122762 (2021). DOI: 10.1016/j.jchromb.2021.122762.

7 For more information see: https://www.helsinki.fi/en/projects/gidprovis.

8 See: (a) O. Anttalainen, E. Lattouf, et al. Review of Scientific Instruments 92, 054104 (2021). DOI: 10.1063/5.0050669; and (b) E. Lattouf, O. Anttalainen, et al. J. Am. Soc. Mass Spectrom., 32, 2218 (2021). DOI: 10.1021/jasms.1c00158.

effects of sulfur mustard on DNA, but that this topic is under consideration for future exploration; this would likely be done by looking into the effect exposure has on marine life, such as fish and other sea organisms. Regarding the presence of sulfur mustard conjugation products or degraded conjugation products in urine, Prof Vanninen indicated that it is not yet known if these products are excreted in urine, but they can be detected in urine matrices, as this has been successfully performed with spiked samples.

7.8 The Board also discussed the importance of continued research in high throughput sampling and analysis. It was noted that in any investigation into the use of a chemical weapon, or ensuring the absence of a toxic chemical following remediation, a statistics-based approach that leads to high confidence in the results is important. This necessitates the ability to collect and analyse many samples, ideally without destroying the samples. The SAB believes this is a highly relevant field that deserves more attention moving forward.

8. AGENDA ITEM EIGHT – Capacity-building programmes of the Technical Secretariat in support of the peaceful uses of chemistry under the implementation of Article XI of the Chemical Weapons Convention

8.1 Mr Sergey Zinoviev, who works in the International Cooperation Branch (ICB) within the International Cooperation and Assistance (ICA) Division of the OPCW, provided the Board with an update on the work of ICB over the past year. He began by giving an overview of Article XI of the Convention and highlighting some of the key aspects, while focusing on the passage indicating that chemistry should be used for peaceful purposes. In that context, the Branch has three thematic areas: integrated chemicals management, promoting chemical knowledge, and enhancing laboratory capabilities.[9]

8.2 In terms of integrated chemicals management, ICB provides training courses on chemical safety and security management, Responsible Care®, and green and sustainable chemistry, among other topics. The Branch also runs an Associate Programme which is a nine-week course offered once per year, in which participants receive lectures, partake in practical exercises, and conduct small training projects at industry sites. All ICB training activities fit into an overarching 360-degree approach, covering chemical safety and security to countering chemical terrorism.

8.3 ICB also has a series of activities aimed at promoting the exchange of chemical knowledge. The Fellowship Programme provides young professionals with on-the-job training at advanced laboratories. There are also opportunities to receive financial support, either to conduct research related to the implementation of the Convention, or to participate in international conferences, seminars, or workshops in fields related to the Convention. There are also more focused opportunities, such as Peaceful Uses of Chemistry for Youth, or Women in Chemistry, among others.

8.4 There are also a number of training and capacity-building opportunities centred around laboratory capabilities. These include laboratory twinning and assistance, training to better prepare laboratories for OPCW proficiency tests, and specialised laboratory training, as needed. There is even an equipment exchange programme where the OPCW will facilitate the transfer of unneeded laboratory equipment from developed economies to those that are developing or in transition.

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9 A more detailed description of Article XI programmes can be found here: https://www.opcw.org/resources/capacity-building.

8.5 Lastly, a brief overview was given on the upcoming activities for the rest of 2022. Mr Zinoviev noted the continued assistance that SAB members have provided for ICB training courses and thanked the Board for its efforts. adding that the cooperation is highly valued. The floor was then opened for questions.

8.6 The Board noted that from a medical point of view, the early detection and prevention of exposure to toxic chemicals—whether related to chemical weapons or in an environmental context—is important. Mr Zinoviev reminded the Board that ICA does address medical countermeasures as part of its Article X activities. They also partner with Responsible Care® to provide chemical safety and security training courses. He also mentioned the Branch offers a series of activities related to green chemistry under Article XI that also cover this topic.

8.7 The Board appreciates that it is able to participate in the process to review research proposals received under Article XI through two nominated Board members. It queried how the SAB can further assist this process to ensure that this programme delivers the maximum impact. Mr Zinoviev noted that the Secretariat always issues Notes announcing opportunities as they arise, and that these are sent to National Authorities. However, they continue to try to reach the scientific communities directly and more effectively. He asked for the Board's help in disseminating and communicating these research grant opportunities.

8.8 Mr Zinoviev was also asked what steps the Secretariat is taking towards establishing partnerships for chemical safety and security training courses focused on manufacturers in States Parties with significant chemical industries. He reminded the Board of the recent document entitled "Indicative Guidelines for Chemical Safety and Security in Small and Medium-sized Enterprises to Foster the Peaceful Uses of Chemistry",[10] which was published to help industrial partners identify and implement best practices in chemical safety and security. However, the Secretariat is always looking for additional partnerships to strengthen its chemical safety and security management programme and welcomes any additional thoughts or ideas the SAB may have in this regard.

9. AGENDA ITEM NINE – Update on the Temporary Working Group on the Analysis of Biotoxins

9.1 Dr Crister Åstot, the chair of the Temporary Working Group (TWG) on the Analysis of Biotoxins, provided the Board with an update of the TWG's progress. He noted that the TWG held its first in-person meeting—and fifth overall—in June, the week following the SAB's last session. The group will hold its sixth meeting in person in October 2022.

9.2 The TWG has made great progress towards fulfilling its mandate. Dr Åstot gave a brief overview of the status of the work of each of the five subgroups, which consider the different questions set out in the TWG's terms of reference, indicating that after the upcoming sixth meeting, the group will shift its focus to producing its end-of-mandate report, which will include a list of appropriate recommendations. He also noted the SAB's appreciation for the European Union's provision of funding for the TWG.

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[10] The entire set of guidelines is accessible at the following link: https://www.opcw.org/sites/default/files/documents/2021/06/OPCW%20Indicative%20Guidelines%20CSSM%2029062021%20Final_1.pdf.

9.3 The Board asked to what extent bioregulators were considered in the work of the TWG. Dr Åstot replied that indeed the TWG has been considering these types of compounds, but there is a paucity of publicly available information on them.

10. AGENDA ITEM TEN – Updates from the Verification Division

10.1 Ms Carolyn Browne (Director of the Verification Division) discussed some of the current activities and considerations within the Verification Division.

10.2 The Director of Verification mentioned several topics that the Division has noted as important in the context of the upcoming Fifth Review Conference. One major change since the Fourth Review Conference has been how the Secretariat has been more effective and efficient in enacting its mandate related to declaration and verification information and data. She also noted the disparity between the verification and inspection mandates in the Convention on the one hand, and the current realities in the chemical industry on the other hand; growth and change in the industry has been extensive since the entry into force of the Convention. This is particularly true for Schedule 2.B4 and other chemical production facilities. This makes site selection more and more challenging. For all matters related to Article VI inspections, the Industry Cluster remains a relevant forum to appropriately bring up considerations and discuss paths forward.

10.3 An update was also provided on the anticipated and scheduled completion of the destruction of declared chemical weapons. Another topic of increasing interest is sea-dumped chemical weapons. The Secretariat has recently clarified to States Parties the mandates in the Convention related to sea-dumped chemical weapons, actions that the Secretariat have taken in this area, and what facilities the Secretariat could offer if a State Party were interested in further discussion or assistance.

10.4 After Ms Browne concluded, the SAB asked several clarifying questions. One was related to the future expectations for inspections, including aspects of sampling and analysis following a gap in their scheduling during the COVID-19 pandemic. Ms Browne noted that the Secretariat is currently ascertaining the frequency with which these can and should occur moving forward based on the benefits they bring and the necessary agreements with States Parties, in addition to the increased complexity and costs entailed.

11. AGENDA ITEM ELEVEN – Scientific report to the Fifth Review Conference – Subgroup breakout sessions

The SAB separated into predefined subgroups to better cover the various topics being considered in the context of its scientific report. Working in smaller groups made it possible to more expediently draft text, advice, and recommendations, which could subsequently be more quickly considered by the entire Board for adoption. The Board held breakout sessions several times throughout this SAB session.

12. AGENDA ITEM TWELVE – Insects as environmental samplers

12.1 Insects have been around for approximately 300 million years and are extremely ubiquitous, being found in almost all areas of the globe. There are almost 1,200 species of blow fly, and this type of fly can be very useful forensically. In particular, given the very predictable timelines of blow fly reproduction and larval growth, times of death of cadavers can be fairly accurately determined and often assist in time-of-death investigations. There has also been a growing interest in using insects as chemical sensors.

12.2 Prof Christine Picard (Indiana University–Purdue University Indianapolis) and her research group have been looking not at what chemicals blow flies sense, but rather what chemicals blow flies ingest, as this may yield information related to their movements. Blow flies have some attractive attributes in that they can travel 10 – 15 km in a day and can be easily baited for collection. After giving an overview of the current field of insect sensing, Prof Picard presented her group's current research into understanding the persistence of chemical weapons agent simulants in blow flies as environmental samplers.

12.3 For this research, Prof Picard's group focuses on detecting and identifying the pentavalent phosphorus moiety that is often at the core of many nerve agents. Initial experiments indicated that after just a few hours of exposure to phosphorus-containing chemicals in faecal matter, associated metabolites in the guts of blow flies could be detected even after two weeks.[11] She also indicated that her group is planning experiments to understand the maximum length of time these compounds are still detectable, noting that the lifespan of an average blow fly can vary from three to 12 weeks.

12.4 Part of the group's research entailed developing the best techniques and associated methods to both sample and analyse samples from the digestive systems of blow flies. They developed and validated a method based on liquid chromatography-mass spectrometry/mass spectrometry (LC-MS/MS) that allowed them to detect and identify a range of chemical weapons agent simulants and hydrolysis products in fly matrix.[12] The compounds tested include dichlorvos, diisopropyl methylphosphonate (DIMP), diethyl phosphoramidate (DEPA), dimethyl methylphosphonate (DMMP), ethyl methylphosphonic acid (EMPA), isopropyl methylphosphonic acid (IMPA), and pinacolyl methylphosphonic acid (PinMPA). To ensure that detection and analysis is possible in the field, they also are developing an approach that combines surface enhanced raman spectroscopy (SERS) with paper-spray MS. This involves developing and testing custom sampling materials that are appropriate for both analytical techniques. This combination allows them to use two portable orthogonal techniques to identify the same chemical weapon agent simulants of interest. In addition to the development of this analytical method, numerous studies have been conducted to understand the effects that the ingestion of these toxic chemicals has on the health and biology of blow flies upon exposure to different concentrations of these chemical warfare agent simulants in various environments.

12.5 Prof Picard concluded by saying that blow flies appear to preserve chemical weapons agent simulants (and some hydrolysis products) in their guts under a wide array of environmental conditions. While these are only the first steps in understanding how blow flies may be used as environmental samplers, it could be possible to target a specific area to extract chemical information from the environment based on blow fly sampling and subsequent analysis. The next steps that Prof Picard's research team is taking include looking into sampling of insensitive munitions to potentially determine their locations, better understanding fly behaviours to better understand their flight patterns and where they have been more accurately, and developing techniques to streamline the detection of blow fly guts in order to remove the dissection step.

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11 C. G. Owings, C. Skaggs, et al. Environ Entomol. 47(3): 586 593 (2018). DOI: 10.1093/ee/nvy027.

12 S. N. Dowling, C. L. Skaggs, et al. Environ. Sci. Technol. 56, 6, 3535–3543 (2022). DOI: 10.1021/acs.est.1c07381.

12.6 Prof Picard was asked whether there have been any studies in which trackers have been attached to flies that were then marked and directed to certain places to sample (eat) and then return to a known location. She indicated that this would be challenging as it is difficult to direct a fly. However, one could release them in a particular desired environment to be sampled, and they could be baited to a known location after a certain time period for analysis.

12.7 The Board also wondered whether ingested chemicals clear out after a certain time simply as part of their normal digestive functions. Prof Picard indicated they have not looked at whether the presence of compounds in the gut would be lengthened if the flies were starved or fed more to impact their digestive functions.

12.8 The Board also commented that if it were known what levels of exposure killed the flies, the presence of dead flies would be indicative of a release or other exposure of a toxic chemical. The dead flies could then be collected and analysed to determine the toxic chemical that killed them. Prof Picard added that while these experiments have not been conducted, it would be interesting to understand the efficacy of the approach.

13. AGENDA ITEM THIRTEEN – Interlaboratory comparison study of a chemical profiling method of methylphosphonic dichloride, a nerve agent precursor

13.1 By-products are always formed in the production of chemical warfare agents. These impurities—in addition to impurities carried through the synthesis from the precursor chemicals—could provide information about how a particular chemical warfare agent was produced. These can be referred to as chemical attribution signatures. However, while a chemical attribution profile can be obtained for any given synthesized chemical, specificity and reproducibility in the analysis of the profile will determine just how useful this kind of attribution profile can be.

13.2 Board member Dr Crister Åstot (Swedish Defence Research Agency (FOI)) presented some of the work his team has done in an interlaboratory study on determining and comparing the attribution profile of methylphosphonic dichloride (DC), a key precursor in the synthesis of sarin.[13] The team used standard gas chromatography-mass spectrometry (GC-MS) methods across eight different laboratories—many of which are OPCW designated laboratories—to understand the potential to use the chemical attribution profile of DC to provide information related to the provenance of a given sample of sarin. FOI took the lead for the overall study, with other laboratories participating to different extents.

13.3 Both FOI and VERIFIN completed an initial study to determine the best GC column to use for analysis, and also developed a methodology for everyone to follow for the workup of test samples. Two other laboratories, Pacific Northwest National Laboratory (PNNL) and a laboratory of the direction générale de l'armement (DGA), joined as organisers and helped in the synthesis of DC using two different methods, the selection of the chemical attribution signatures to focus on, and the development of the reference sample. The various samples were then analysed with GC-MS instruments by these four laboratories plus an additional four laboratories, and FOI then analysed all the data collected.

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13 K. H. Holmgren, H. Hakulinen, et al. Interlaboratory Comparison Study of a Chemical Profiling Method of Methylphosphonic Dichloride, a Nerve Agent Precursor. Available at SSRN: http://dx.doi.org/10.2139/ssrn.4269900.

Hierarchical clustering of the collected data showed that the synthetic procedure used can be determined by looking at the chemical attribution signatures that are present, regardless of which laboratory did the analysis. The study found 2 – 3 major signatures, and 13 – 14 minor signatures for each of the two synthetic methods used. Dr Åstot indicated the team is currently preparing a manuscript to submit for publication.

13.4 Upon being asked whether impurities present in the raw materials and precursors used in the syntheses were considered, Dr Åstot replied that they were not a focus for these experiments; the focus was on the by-products generated during synthesis, not the impurities that were already present in the starting materials.

14. AGENDA ITEM FOURTEEN – Route attribution of sulfur mustard using non-targeted chemical attribution signature screening

14.1 Dr Åstot then presented the results of other work being done at FOI to better understand the route attribution of sulfur mustard. They looked at 11 different routes for the production of sulfur mustard and conducted analyses with both GC-MS electron ionisation (EI), a low-resolution technique, and high-resolution (HR)MS EI. They found that the low-resolution GC-MS method allowed them to classify the sulfur mustard samples according to the method used in the last step of the synthesis, identifying 103 chemical markers. However, a more sensitive and selective technique was needed to elucidate the chemical markers indicative of earlier steps in the synthesis.[14]

14.2 The FOI team then used GC-HRMS and were able to differentiate between all 11 of the synthetic routes used by identifying and elucidating the chemical attribution signatures in the synthesis of thiodiglycol, a direct precursor to sulfur mustard.[15] They challenged their methodology by spiking small amounts of sulfur mustard sample in both soil and textile samples. They saw that while many new chemical attribution signatures were formed in the resulting samples, they could still identify many signatures that were independent of the matrix used.

14.3 A robust discussion followed, in which Dr Åstot was able to provide additional context for the work presented. The Board noted the challenges associated with chemical profiling work, i.e., the myriad of samples required and the subsequent detailed analysis of data needed to try to identify and determine the best chemical attribution signatures to use. The field of chemical profiling is still relatively new. It was asked whether any thought has been given to identifying new ways to efficiently generate more samples and collect more data to populate machine-learning models. Dr Åstot noted that there are a number of inherent challenges in chemical profiling. One is the importance of the appropriate reference samples for a ground truth baseline. Another is that while synthetic conditions can be varied to collect more data, the conditions associated with authentic samples are likely not known *a priori*, and so these will limit the utility and ability to try to pre-emptively generate useful models. In addition, there is still the issue of standardising methods and approaches among different laboratories, an issue that is complex in and of itself.

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14 K. H. Holmgren, S.Hok, et al. Talanta, Vol 186: 615-621 (2018). DOI: 10.1016/j.talanta.2018.02.100.

15 K. H. Holmgren, L. Mörén, et al. Analytical Chemistry, 93 (11), 4850-4858 (2021). DOI: 10.1021/acs.analchem.0c04555.

14.4 It was further noted that there is another aspect to chemical profiling that is important to remember: its utility in retrosynthesis, i.e., reconstructing a synthetic approach. For example, if there are multiple attacks with a chemical warfare agent, then chemical profiling could be used to aid in the retrosynthesis of the agents to indicate whether they were produced the same way, or in the same laboratory or batch. This information could, for example, help determine whether multiple attacks could be attributed to a single perpetrator or not.

14.5 The Board observed that other analytical tools in addition to the MS approaches highlighted in these presentations, such as nuclear magnetic resonance spectroscopy or ion chromatography, may provide further useful information for a given sample or situation. Similarly, the analysis of signatures not directly related to the chemical warfare agents themselves could be useful, such as impurities present in starting materials or introduced from storage conditions, for example.

15. AGENDA ITEM FIFTEEN – Discussion with the Declaration Assessment Team

15.1 The Head of the DAT, Mr Nihad Alihodzic, along with an expert from the team, Mr Moez Hani, gave an overview of the work of the DAT. The DAT was established by the Director-General in 2014 with the mandate to verify whether the declaration submitted by the Syrian Arab Republic is accurate and complete, as required under the Convention, relevant decisions of the OPCW policy-making organs, and United Nations Security Council resolution 2118 (2013). The DAT engages with the relevant Syrian authorities to resolve the identified gaps, inconsistencies, and discrepancies noted by the Secretariat in the Syrian Arab Republic's declaration regarding its chemical weapons programme upon signing and ratifying the Convention in 2013.

15.2 In order to better understand and validate some of the explanations of declaration-related issues provided by the Syrian authorities, in 2016 the DAT started its chemical profiling work by trying to reconstruct the history of chemicals identified in authentic samples dating back to 2014.

15.3 In this context, the DAT explained the complexity and challenging aspects of this work in light of the following factors, among others: the Syrian chemical weapons programme spanned over four decades; there are no ready-made tools or approaches; the fact that the complete environmental conditions and subsequent ageing and/or degradation of the collected samples are unknown; multiple synthetic methods were used for the production of chemical warfare agents and their precursors; and the enormous variability in the concentrations and types of chemicals present in the samples. All these factors may be important to understand the provenance of the chemicals identified in the samples.

15.4 The DAT also underlined that the information relevant to chemical profiling of authentic samples is not limited to the data provided by designated laboratories. Additional relevant information may come from various other sources, including documents, information gathered through technical meetings, interviews, photos, videos, or from other sources. This information remains critical to providing additional context to chemical samples and their analysis, and for understanding the entire situation as a whole and the context in which the chemical profiling is to be conducted. As such, the DAT emphasised the fact that chemical profiling of authentic samples shall be conducted with prior knowledge of all other information related to the case.

15.5 Due to the difficulties and complexities named above, the DAT has applied a broader approach from how the OPCW, and the designated laboratories, usually analyse samples in the proficiency testing context. Accordingly, the DAT has identified additional needs, such as the need to broaden the scope of analysis of authentic samples and have access to all data generated by the designated laboratories during the analysis of these samples. This approach is time consuming, and collecting and managing the data is labour intensive. Given the breadth of data, and noting the sensitivity associated with authentic samples, the DAT noted that full automation of the process is difficult, thereby initially necessitating a very hands-on, manual approach to ensure correctness and validity. In spite of the complexity of the data, the DAT managed to automate a few segments of the whole process, which will be further tested in the future.

15.6 The DAT's work demonstrates the potential complexity of real cases that need further investigation beyond the standard question of identifying whether or not a scheduled chemical is present in a given sample. The DAT is looking to share the lessons it has learned and approaches to collection and analysis both within and outside the Secretariat so that others may benefit, and to ensure that the Secretariat remains capable of addressing similar situations in the future.

15.7 After the presentation, Mr Alihodzic and Mr Hani answered several questions from the Board related to some of the specifics of their approach and methodology, as well as how samples are collected and analysed.

16. AGENDA ITEM SIXTEEN – Update on recent Scientific Advisory Board workshops and planning for future events

16.1 Before discussing potential future topical workshops and events, brief synopses were given on the two topical workshops the Board held immediately after its Thirty-Fifth Session in June. These workshops were important in providing the Board with a deeper understanding of some of the most pertinent topics to be addressed in its scientific report.

16.2 First, the SAB Secretary, on behalf of Board member Prof Ahmed Saeed, shared the main points from the SAB-IUPAC workshop on artificial intelligence (AI)-assisted chemistry, held on 16 and 17 June 2022 at the OPCW Headquarters. The workshop provided insight into current and future applications of AI in chemistry by addressing topics such as utility in synthetic design, reaction conditions and optimisation, agricultural chemistry, drug discovery, the potential impact of AI on the chemical industry, and potential implications for IUPAC and the OPCW. The objectives of the workshop were to not only provide IUPAC and the OPCW with an update on the various research approaches and the state of the art in AI-assisted chemistry, but to also generate provocative discussions on the future of the field and potential positive and negative impacts it may have on the chemical sciences and on society as a whole. To that end, workshop participants included members of the SAB, Secretariat staff, representatives from IUPAC, and invited external speakers. The workshop featured seven speakers representing industry and academia and included several moderated discussion sessions that delved into some of the important themes the speakers presented.[16]

[16] The workshop agenda can be found as Annex 2 of this report.

16.3 A rich discussion followed on dual-use science and how scientists and researchers can be better attuned to the potential dual-use nature of their research and publications they may produce. More can be done to educate and raise awareness in the scientific community, but there will always be a challenge in balancing academic and research freedom with safety and security concerns. The Board proposed holding a workshop in the near future focused on emerging technologies.

16.4 A second topical workshop was held at the BASF facility in Antwerp on 20 and 21 June 2022. This workshop, held collaboratively with the chemical industry, focused on emerging scientific trends and directions in the chemical industry. Dr Renate Becker-Arnold and Prof Syeda Sultana Razia, the two Board members who took the lead in organising the workshop, presented an overview of the workshop and the important takeaway points. The workshop featured presentations by nine invited speakers, with eight representing industry and one from a non-governmental organisation.[17] Other participants included SAB members and Secretariat staff. Topics discussed included digitisation in the chemical industry, green chemistry and the circular economy, and emerging technologies, processes, and sustainability. The rich and extensive discussions ensured that the Board gained a better understanding of some of the important innovations and directions that the industry is investigating and potentially incorporating. Participants also took a tour of the BASF facility to gain a better understanding of the production processes used and the infrastructure required.

16.5 The SAB then discussed upcoming events that are important to the Board's work. Of particular note is the upcoming 52nd IUPAC General Assembly (18 – 25 August 2023) and the 49th IUPAC World Chemistry Congress (20 – 25 August 2023) taking place in The Hague, the Netherlands. The Board discussed several ways in which it can collaborate with IUPAC to participate in this conference.

17. AGENDA ITEM SEVENTEEN – Discussion on central nervous system-acting chemicals

As part of its standard process in preparing its scientific report, the Board considered what advice to give, and recommendations to make, with regard to central nervous system-acting chemicals.

18. AGENDA ITEM EIGHTEEN – Update on cooperation with chemical industry associations and preparatory work for the Fifth Review Conference focusing on verification-related issues under Article VI

18.1 Mr Szymon Bochenski (Senior Policy Officer in the Office of Strategy and Policy) provided an update both on the Secretariat's ongoing cooperation with the chemical industry and on the preparations for the Fifth Review Conference, with a focus on verification-related issues.

18.2 In line with the recommendations issued at the Third Review Conference, the OPCW has continued to strengthen relations with the chemical industry, at both the regional and international levels. Cooperation was formalised with the International Council of Chemical Associations in 2015, and with the International Chemical Trade Association more recently in 2020. The OPCW engages with these partners via the Chemical

[17] The workshop agenda can be found as Annex 3 of this report.

Industry Coordination Group, which meets twice a year. The OPCW and its industry partners exchange information, discuss steps to improve industry inspections, and notify each other of capacity building on chemical safety and security and peaceful uses of chemistry. More recent discussion has focused on collaboration related to science and technology, and led to cooperation on the SAB-Industry workshop that was held in June 2022.

18.3 The upcoming Review Conference provides a forum to assess the operation of the Convention, reaffirm collective understandings, address challenges encountered in the full implementation of the Convention, provide guidance on further operation of the Organisation, and consider advances in science and technology. Mr Bochenski provided an overview of how the Secretariat and the OPCW are preparing for the Fifth Review Conference. Of particular note for the SAB is the briefing on science and technology scheduled for 2 November 2022, at which the Chairperson of the SAB and the OPCW Science Policy Adviser addressed States Parties and provided a synopsis of the SAB's work over the past five years, to include an overview of its forthcoming report.

19. AGENDA ITEM NINETEEN – Specialised Article VI programming on verification-related issues

19.1 The Implementation Support Branch (IPB) is responsible for coordinating activities intended to support and sustain the capacities of States Parties and their National Authorities for the full and effective implementation of the Convention. The Branch provides tailored assistance, training, and capacity-building activities to assist States Parties in their implementation of the Convention. Mr James Pettit (Programme Officer, IPB) provided an overview of the IPB's training on Article VI, including general training courses on obligations under the Convention, courses on declarations and inspections under Article VI of the Convention, and training-of-trainers courses for representatives of customs institutions. He noted that among other things, the Branch is currently looking to implement more specialised programmes for States Parties with significant declarable activity under Article VI.

19.2 Very recently, the IPB held a pilot forum on verification issues for States Parties with Schedule 2 plant sites in close collaboration with the Verification Division. This was a new activity that provided States Parties an opportunity to engage with the Secretariat on relevant verification issues related to Schedule 2 plant sites. It also provided a forum for participants to exchange information and good practices with each other and discuss the changing nature and future of Schedule 2-related industry. The pilot forum was attended by 28 delegates from 17 States Parties and has received positive initial feedback. The IPB will continue to consult with delegates that attended in order to receive comprehensive feedback and better understand the impact of the workshop and possible next steps.

19.3 The Board asked for a further description of the customs training courses. Mr Pettit explained that they use a training-of-trainers model whereby States Parties nominate representatives from their customs training institutions, and these participants receive training on declarations obligations relevant to customs, and then integrate the knowledge gained into their own customs training programmes. The way in which this new knowledge is integrated into national training programmes varies, but the training is not prescriptive; each trained participant, knowing their own country's approach, should utilise the information in a way appropriate for their situation.

20. AGENDA ITEM TWENTY – Election of the Scientific Advisory Board Chairperson and Vice-Chairperson

20.1 The Board, with the assistance of the SAB Secretary, held a private meeting to elect its Chairperson and Vice-Chairperson for 2023. No interpretation was provided, and only Board members physically present were in attendance. Mr Günter Povoden and Dr Andrea Leisewitz were both re-elected, by consensus, to continue serving as Chairperson and Vice-Chairperson, respectively, in the next year.

20.2 After the election, the Board recognised and paid tribute to its two Board members whose tenure will finish at the end of 2022, Dr Renate Becker-Arnold and Prof Ahmed Saeed. Their efforts over their six years with the SAB have been exemplary and the entire Board wishes them all the best in the future.

21. AGENDA ITEM TWENTY-ONE – Plenary discussion on the scientific report

After working in their various subgroups throughout the week, the Board deliberated the initial major text and recommendations proposed by each of the subgroups. After doing an initial pass through all the text, with the opportunity for any Board member to make comments or suggestions, the ideas for the main recommendations were agreed upon. The Board decided to continue working on the document in correspondence with a goal of finishing the entire report by the end of November 2022, considering the iterative process of the report and the recommendations therein, as well as the need to receive input and agreement from the Board members not present.

22. AGENDA ITEM TWENTY-TWO – Any other business and closing remarks

22.1 The floor was opened for any other business. Upon receiving no requests for the floor, the Chairperson thanked the Secretariat staff, the interpretation team, and all the Board members for their assistance and participation throughout the session.

22.2 The SAB is grateful to all States Parties, organisations, and institutions that have financially assisted the work of the Board.

23. AGENDA ITEM TWENTY-THREE – Adoption of the report

The SAB agreed to adopt the report for its Thirty-Sixth Session via correspondence after the session.

24. AGENDA ITEM TWENTY-FOUR – Closure of the session

The Chairperson closed the session at 17:58 CET on 29 September 2022.

Annex 1:	List of Participants in the Thirty-Sixth Session of the Scientific Advisory Board
Annex 2: (English only)	Agenda of the Workshop on Artificial Intelligence-Assisted Chemistry
Annex 3: (English only)	Agenda for the OPCW SAB-Industry Collaborative Workshop on Emerging Scientific Trends and Directions in the Chemical Industry

Annex 1

LIST OF PARTICIPANTS IN THE THIRTY-SIXTH SESSION OF THE SCIENTIFIC ADVISORY BOARD

	Participant	Institution
Members of the Scientific Advisory Board		
1.	Dr Crister Åstot	Swedish Defence Research Agency (FOI), Sweden
2.	Dr Khaldoun Bachari	Algerian Public Scientific and Technical Research Centre in the Physico-Chemical-CRAPC, Algeria
3.	Dr Renate Becker-Arnold	BASF, Germany
4.	Dr Elma Biscotti	Scientific and Technical Research Institute for Defense, Argentina
5.	Dr Anne Bossée	DGA CBRN Défense, France
6.	Prof Vladimir Dimitrov	Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Bulgaria
7.	Mr Raza Ellahi	Defence Science & Technology Organization (DESTO), Pakistan
8.	Prof Mostafa Ghanei, MD	Baqiyatallah University of Medical Sciences, Iran (Islamic Republic of)
9.	Dr Norman Govan	Defence Science and Technology Laboratory, United Kingdom of Great Britain and Northern Ireland
10.	Dr Matteo Guidotti	Institute of Chemical Sciences and Technologies (SCITEC) of the Italian National Research Council, Italy
11.	Prof Victor Kholstov	Ministry of Industry and Trade, "GosNIIOKhT", Russian Federation
12.	Mr Wilford Jwalshik	Institute of Chartered Chemists, Nigeria
13.	Dr Robert Kristovich	United States Army DEVCOM Chemical Biological Center, United States of America
14.	Dr Andrea Leisewitz (Vice-Chairperson)	Universidad San Sebastián, Chile
15.	Prof Imee Su Martinez	University of the Philippines-Diliman, Philippines
16.	Prof Elisa Souza Orth	Federal University of Paraná, Brazil
17.	Mr Günter Povoden (Chairperson)	CBRN Defence Centre, Ministry of Defence, Austria
18.	Prof Ines Primožič	University of Zagreb, Croatia
19.	Prof Syeda Sultana Razia	Bangladesh University of Engineering and Technology (BUET), Bangladesh
20.	Prof Ahmed E. M. Saeed	Sudan University of Science and Technology, Sudan
21.	Dr Maciej Sliwakowski	Lukasiewicz Research Network – Institute of Industrial Organic Chemistry, Poland
22.	Prof Fengxia Sun	Hebei University of Science and Technology, China

Invited Participants		
23.	Mr Nihad Alihodzic	Organisation for the Prohibition of Chemical Weapons, Netherlands
24.	Mr Szymon Bochenski	Organisation for the Prohibition of Chemical Weapons, Netherlands
25.	Dr Carolyn Browne	Organisation for the Prohibition of Chemical Weapons, Netherlands
26.	Mr Moez Hani	Organisation for the Prohibition of Chemical Weapons, Netherlands
27.	Mr James Pettit	Organisation for the Prohibition of Chemical Weapons, Netherlands
28.	Prof Christine Picard	Indiana University–Purdue University Indianapolis, United States of America
29.	Prof Paula Vanninen	VERIFIN, Finland
30.	Dr Sergei Zinoviev	Organisation for the Prohibition of Chemical Weapons, Netherlands
Secretary to the Scientific Advisory Board		
31.	Dr Peter Hotchkiss	Organisation for the Prohibition of Chemical Weapons, Netherlands

Annex 2

**AGENDA OF THE WORKSHOP
ON ARTIFICIAL INTELLIGENCE-ASSISTED CHEMISTRY**

	Thursday 16 June 2022
15:00	Overview of artificial intelligence-assisted chemistry workshop (Prof Ahmed Saeed and SAB Secretary)
15:30	AI in drug discovery: Avoiding doing more harm than good (Sean Ekins, Collaborations Pharmaceuticals, Inc.)
16:30	*Break*
17:00	Artificial, augmented, and automated chemistry (Prof Jeremy Frey, University of Southampton)
18:00	Workshop ends for day
	Friday 17 June 2022
09:00	Use of neural networks and symbolic AI in chemical synthesis planning (Dr Marwin Segler, Microsoft)
10:00	Application of artificial intelligence in agricultural chemistry and agriculture (Dr Bipulbehari Saha, Sagar Group of Institutions)
11:00	*Break*
11:15	Self-optimising reactors for industry 4.0 process development (Prof Richard Bourne, University of Leeds)
12:15	Moderated discussion
13:00	*Lunch*
15:00	Sustainability implications of AI in the chemical industry (Prof Yuan Yao, Yale University (virtual presentation))
16:00	Use of AI in molecular design, reaction planning, and reaction execution (Prof Connor Coley, MIT (virtual presentation))
17:00	*Break*
17:15	Moderated discussion
18:00	Workshop ends

Annex 3

AGENDA OF THE OPCW SAB-INDUSTRY COLLABORATIVE WORKSHOP ON EMERGING SCIENTIFIC TRENDS AND DIRECTIONS IN THE CHEMICAL INDUSTRY

	Monday 20 June 2022
09:00	Participant arrival and room set-up
09:30	Opening of the workshop (Renate Becker-Arnold, Syeda Sultana Razia, Peter Hotchkiss)
10:00	Session 1: Digitisation in the chemical industry (with intermission) • Digitisation in the chemical industry (Catharina Müller-Buschbaum, Accenture GmbH) • Cyber Security Deep Dive (Volker Wagne, BASF) • Digital traceability in a blockchain infrastructure (Heinz-Günter Lu, Evonik) • Monitoring and tracking chemicals (MATCH) prototype: using blockchain to track chemical transfers (Cindy Vestergaard, Stimson Center)
13:00	*Lunch*
14:30	Moderated discussion
15:45	*Break*
16:15	Session 2: Green chemistry and the circular economy • Circular Economy in the chemical industry (Bernhard Ulrich von Vacano, BASF) • Safe and sustainable by design (Ann Dierckx, CEFIC)
17:45	End of day 1
	Tuesday 21 June 2022
09:00	Session 3: Emerging technologies, processes, and sustainability • Principles in process safety: an overview (Hagen Weig, BASF) • New biotech processes and the impact on global chemical supply chains (Doreen Schachtschabe, BASF) • Chemical industry: a driver for sustainability (Detlef Männig, Mannig Consulting)
10:45	*Break*
11:15	Moderated discussion
12:15	Final thoughts / recap
12:30	*Lunch*
13:30	Introduction to site BASF Antwerpen N.V. and tour of BASF facility
16:00	End of workshop

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